I. Ground States in Quantum Mechanics

A. Quantization of Newton's Equations

* In classical mechanics one considers systems $m\ddot{x} = -\nabla V(x)$ for curves $x(t): I \to \mathbb{R}^d$, $I \subseteq \mathbb{R}$ an interval, and $V(x): \mathbb{R}^d \to \mathbb{R}$.

* one has conservation of energy $E = \frac{1}{2}m|\dot{x}|^2 + V(x)$.

* One makes this into an ODE via $\xi = m\dot{x}$, then $E = \frac{1}{2m}|\xi|^2 + V(x)$ where $\dot{x} = \frac{1}{m}\xi = \partial_\xi E$, $\dot{\xi} = -\nabla_x V = -\nabla_x E$ (Hamilton's Eq).

* The quantum mechanical version of this is to evolve the "wave function" $\phi(t) \in \mathcal{H} = L^2(\mathbb{R}^d)$ according to $i\hbar\partial_t\phi = \frac{-\hbar^2}{2m}\Delta_{\mathbb{R}^d}\phi + V(x)\phi$ so the energy of the system is $E\{\phi(t)\} = \int_{\mathbb{R}^d}\left(\frac{\hbar^2}{2m}|\nabla\phi|^2 + V(x)|\phi|^2\right)dx$. For this problem $\|\phi(t)\|_{L^2} \equiv \text{const}$ ($V \in \mathbb{R}$), so normalizing $\|\phi\|_{L^2} = 1$ we have $|\phi(t)|^2 dx = \mu$ & $\frac{1}{(2\pi)^d}|\hat{\phi}(t)|^2 d\xi = \nu$ are the probability densities for particle position and momentum.

B. Standing waves and bound states.

* We now look for special solutions of $i\hbar\partial_t\phi = -\hbar^2/2m\,\Delta\phi + V\phi$ which are of the form $\phi(t,x) = e^{-iE_0/\hbar\, t}\phi_0(x)$. These solve the time independent equation $-\hbar^2/2m\,\Delta\phi_0 + V\phi_0 = E_0\phi_0$. Rescaling x variables $\phi_0(x) = u_0\left(\frac{\sqrt{2m}}{\hbar}x\right)$, $V = Q\left(\frac{\sqrt{2m}}{\hbar}x\right)$ we get $(\Delta - Q)u_0 = -E_0 u_0$.

* We hope to find such u_0 by minimizing the functional $I\{u\} = \int\left(|\nabla u|^2 + Q|u|^2\right)dx$ over $\|u\|_{L^2} = 1$. Indeed, if u_0 is a minimizer with $E_0 = I\{u_0\}$ formally $\frac{d}{d\epsilon}\left(I(u+\epsilon\varphi)/\|u+\epsilon\varphi\|_{L^2}^2\right)\Big|_{\epsilon=0} = 2\int \nabla u_0\cdot\nabla\varphi + Qu_0\varphi - E_0u_0\varphi = 2\int(-\Delta u + Q - E_0)u_0\varphi$ which implies $-\Delta u_0 + Qu_0 = E_0 u_0$ in the sense of distributions.

II. Solution of the variational problem

A. Admissible potentials

* We now discuss the class of potentials for which we expect good minimization.

By Sobolev embeddings we have $\|u\|_p \leq C\|u\|_{H^1}$ for $\begin{cases} 2\leq p<\infty, & d=2 \\ 2\leq p\leq \frac{2d}{d-2}, & d\geq 3 \end{cases}$

* Based on this we get $\left|\int_{\mathbb{R}^d} Q|u|^2\right| \leq C\|Q\|_{P(d)} \cdot \|u\|_{H^1}^2$

when $P(d) = \begin{cases} L^p + L^\infty_0, & d=2 \\ L^{\frac{d}{2}} + L^\infty_0, & d\geq 3 \end{cases}$ where $L^\infty_0 = \{ Q \in L^\infty \mid \lambda_Q(t)<\infty \text{ all } t>0\}$.

This leads us to our first result:

<u>Prop</u>: Let $Q\in P(d)$. Then $I\{u\} = \int |\nabla u|^2 + Q|u|^2$ is well defined, and $\exists$ $C=C(Q)\geq 0$ such that $I\{u\}\geq -C$ all $u\in H^1$ with $\|u\|_{L^2}=1$. In addition I is weakly LSC on H^1 in the sense that if $u_n \rightharpoonup u$ in H^1 one has $I\{u\}\leq \underline{\lim}\, I\{u_n\}$.

<u>pf</u>: Let $Q\in P(d)$, then for every $\epsilon>0$ we can split $Q = Q_\epsilon + \tilde{Q}_\epsilon$ when $\|Q_\epsilon\|_{P(d)}\leq \epsilon$ and $\tilde{Q}_\epsilon \in \mathcal{S}(\mathbb{R}^d)$. Then using Sobolev + Hölder as above $\left|\int Q|u|^2\right| \leq C\epsilon\|u\|_{H^1}^2 + \|\tilde{Q}_\epsilon\|_{L^\infty}\cdot\|u\|_{L^2}^2$. Letting $C\epsilon\leq 1$ we get $I\{u\}\geq -\|\tilde{Q}_\epsilon\|_{L^\infty}\cdot\|u\|_{L^2}^2$.

Similarly, to get the LSC part since $\nabla u_n \rightharpoonup \nabla u$ we know $\int|\nabla u|^2 \leq \underline{\lim}\int|\nabla u_n|^2$. We claim that for $Q\in P(d)$ in fact $\int Q|u_n|^2 \to \int Q|u|^2$. First suppose $Q\in\mathcal{S}(\mathbb{R}^d)$, then this follows by Rellich compactness. In general for $Q\in P(d)$ we write $Q = Q_\epsilon + \tilde{Q}_\epsilon$

Then, $\overline{\lim}\left|\int Q|u_n|^2 - Q|u|^2\right| = \overline{\lim}\int|Q_\epsilon|(|u_n|^2+|u|^2) \leq C\epsilon\,\overline{\lim}(\|u_n\|_{H^1}^2+\|u\|^2)$.

Letting $\epsilon\to 0$ gives the result.

B. Existence of the minimizer

* we now show one can construct a minimum.

<u>Thm</u>: Assume $I\{u\}<0$ for some $u\in H^1$. Then one can find $\|u_0\|_{L^2}=1$ with

$$E_0 = I\{u_0\} = \inf_{\|u\|_{L^2}=1} I\{u\}.$$

<u>pf</u>: Let $E_0<0$ be the infimal value, and $u_n\in H^1$ with $\|u_n\|_{L^2}=1$ and $I\{u_n\}\to E_0$. As above splitting $Q=Q_\epsilon+\tilde{Q}_\epsilon$ as above,
$\|\nabla u_n\|_{L^2}^2 = I\{u_n\}+\int Q|u_n|^2 \leq I\{u_n\}+C\epsilon\|u_n\|_{H^1}^2+\|\tilde{Q}_\epsilon\|_{L^\infty}$. In particular $\|u_n\|_{H^1}\leq C(Q)$ uniformly in n. WLOG assume $u_n\rightharpoonup u_0$ for some $u_0\in H^1$. Then $I\{u_0\}\leq E_0<0$. Thus $u_0\neq 0$. Now if $\|u_0\|_{L^2}<1$, we'd have $I\{w_0\}<E_0$ where $\|w_0\|=1$ by setting $w_0=u_0/\|u_0\|_{L^2}$. Thus $\|u_0\|_{L^2}=1$ and we are done.

* Remark: Note that to get LSC for Q^- Rellich compactness was essential. Also, it is Q^- which provides the "Binding force" which allows $u_0\neq 0$ in the limit. (If $Q\geq 0$ we'd get $u_n\rightharpoonup 0$, i.e. all the mass "escapes" to $|x|\to\infty$).