One-particle systems

Ground state energy. If H is bounded from below, i.e. if $\exists C \in \mathbb{R}$ s.t. $\mathcal{E}(\psi) := \langle \psi, H\psi \rangle \geqslant C \ \forall \psi$, then we define the *ground state energy* $E_0 := \inf\{\mathcal{E}_\psi, \|\psi\| = 1\}$. If there is a minimizer ψ_0 of $\mathcal{E}$, then it is called *ground state* of the system.

Stability of the first kind. The system is called *stable*, if $E_0 > -\infty$. If $\exists K > 0$ s.t. $\int V_- |\psi|^2 \leqslant \|\nabla\psi\|_2^2 + K\|\psi\|_2^2$, then $\mathcal{E}(\psi) \geqslant \|\nabla\psi\|_2^2 - \int V_- \|\psi\|_2^2 \geqslant -K\|\psi\|_2^2$, i.e. this condition on V_- is sufficient for the system being stable.

Condition on V using Sobolev's inequality. Consider $H = -\Delta + V$ and assume $V_- = V_1 + V_2$ where $V_1 \in L^{3/2}$, $V_2 \in L^\infty$. By Sobolev: $\|\psi\|_6 \leqslant C\|\nabla\psi\|_2$. We can assume that $\|V_1\|_{3/2} \leqslant C^{-2}$ (if this does not hold, just cut-off $V_1 = V_1 \mathbb{1}_{V_1 \leqslant M} + V_1 \mathbb{1}_{V_1 \geqslant M}$ and redefine V_2 adding the first term). Then

$$\int V_1 |\psi|^2 \leqslant \|\psi\|_6^2 \, \|V_1\|_{3/2} \leqslant \|\nabla\psi\|_2^2$$

and

$$\int V_2 |\psi|^2 \leqslant \|V_2\|_\infty \, \|\psi\|_2^2$$

Thus the above bound on $\int V_- |\psi|^2$ holds with $K = \|V_2\|_\infty$, so H is stable, if $V \in L^{3/2} + L^\infty$.

Lemma. For $\psi \in M$ and $d \geqslant 2$ we have

$$\int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|} dx \leqslant \|\nabla\psi\| \, \|\psi\|$$

and equality holds only for $\psi_0(x) \propto e^{-c|x|}$. (For the proof, we can calculate $\langle \psi, [\partial_j, \frac{x_j}{|x|}]\psi \rangle$ for $\psi \in C_0^\infty$ in two different ways for: directly and by partial integration, afterwards we use the Schwarz inequality.)

Hardy inequality. For $d \geqslant 3$ and $\psi \in C_0^\infty(\mathbb{R}^d)$

$$\int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|^2} dx \leqslant \frac{4}{(d-2)^2} \|\nabla\psi\|^2$$

(proof as above using the commutator $[\partial_j, \frac{x_j}{|x|^2}]$)

Stability of hydrogen. The ground state energy of hydrogen $E_0 = \inf\{\int |\nabla\psi|^2 - Z \int \frac{|\psi|^2}{|x|} : \psi \in M, \|\psi\| = 1\}$(where $M = \{\psi : \mathbb{R}^3 \to \mathbb{C} : \|\psi\| < \infty, \|\nabla\psi\| < \infty, \int |\psi|^2/|x| < \infty\}$) is given by $E_0 = -Z^2/4$ and $\psi_0(x) = Z^{3/2} e^{-Z|x|/2}/\sqrt{8\pi}$.

Stability of Many-Particle-Systems

Coulomb energy. Let $\boldsymbol{R} \in \mathbb{R}^{Kd}$, $\boldsymbol{Z} = (Z_1, \dots, Z_K)$ with $Z_i > 0$ be given parameters, $V_C(\boldsymbol{x}) := \sum_{k<l} \frac{1}{|x_l - x_k|} - \sum_{j=1}^N \sum_{k=1}^K \frac{Z_k}{|x_j - R_k|} + \sum_{k<l} \frac{Z_k Z_l}{|R_k - R_l|}$, then for $\psi \in L^2(\mathbb{R}^{Nd})$ define $\mathcal{E}(\psi) := \sum_j \int_{\mathbb{R}^{Nd}} |\nabla_j \psi|^2 + \int_{\mathbb{R}^{Nd}} V_C \, |\psi|^2$.

Stability. Set $E_0(\boldsymbol{R}) := \inf\{\mathcal{E}(\psi) | \psi \in M, \|\psi\| = 1\}$, where $M := \{\psi \in L^2(\mathbb{R}^{Nd}) | \int |\nabla_j \psi|^2 < \infty, \int \frac{|\psi|^2}{|x_j - R_k|} < \infty\}$. Then $E_0 := \inf_{\boldsymbol{R}} E_0(\boldsymbol{R}) > -\infty$.

Stability of 2nd kind. A Coulomb system of K nuclei and N electrons satisfies the *stability of 2nd kind*, if $\exists C_Z$ where $Z = \max Z_k$ s.t. $E_0 \geqslant -C_Z(N + K)$.

Summary of analysis

Riesz Fischer theorem. Suppose $1 \leqslant p \leqslant \infty$ and (Ω, μ) is a measure space, then

(i) $(L^p, \|\cdot\|_p)$ is complete.
(ii) If $\|f_n - f\|_p \to 0$, then $\exists (f_{n_k})_k \subset (f_n)_n$ and $F \in L^p$ s.t. $|f_{n_k}(x)| \leqslant F(x)$ and $f_{n_k}(x) \to f(x) \ \forall_\mu \, x \in \Omega$.

Completeness. The following spaces are complete

(i) $C[0,1]$ in $\|\cdot\|_\infty$
(ii) L^∞ in $\|\cdot\|_\infty$
(iii) L^p in $\|\cdot\|_p$
(iv) H^1 is complete in $\langle \cdot, \cdot \rangle_{H^1}$.

Denseness. The following spaces are dense

(i) $C_0^\infty(\Omega) \subset L^p(\Omega)$ is dense in $\|\cdot\|_p$ for $p < \infty$.
(ii) $C_0^\infty(\mathbb{R}^d) \subset H^1(\mathbb{R}^d)$ is dense in H^1-norm.
(iii) $H^1(\Omega) \subset L^2(\Omega)$ is dense in $\|\cdot\|_2$
(iv) The completion of $C[0,1]$ in $\|\cdot\|_p$ is $L^p[0,1]$ for $p < \infty$.
(v) $\{\sum_i c_i \chi_{R_i} | c_i \in \mathbb{C}, R_i \text{ rectangles}\}$ is dense in L^1.

Inequalities.

(i) *Jensen:* Let $J : \mathbb{R} \to \mathbb{R}$ be convex, $\mu(\Omega)$ finite and define for $f \in L^1$: $\langle f \rangle := \frac{1}{\mu(\Omega)} \int_\Omega f d\mu$. Then $\langle J \circ f \rangle \geqslant J(\langle f \rangle)$.
(ii) *Hölder:* For $1 \leqslant p, q \leqslant \infty$ s.t. $\frac{1}{p} + \frac{1}{q} = 1$ we have for $f \in L^p$, $g \in L^q$: $|\int fg \, d\mu| \leqslant \|f\|_p \|g\|_q$.
(iii) *Minkowski:* $\|f + g\|_p \leqslant \|f\|_p + \|g\|_p$ (for $1 \leqslant p \leqslant \infty$)
(iv) *Generalized Minkowski:* $\|\int f(\cdot, y) dy\|_p \leqslant \int \|f(\cdot, y)\|_p dy$.
(v) *Generalized Cauchy-Schwarz:* $|\int fg| \leqslant \frac{1}{2}(\alpha\|f\|_2 + \alpha^{-1}\|g\|_2)$
(vi) *Young:* Let $1 \leqslant p, q, r \leqslant \infty$ with $\frac{1}{p} + \frac{1}{q} + \frac{1}{r} = 2$ then for any $f \in L^p(\mathbb{R}^d), g \in L^q(\mathbb{R}^d), h \in L^r(\mathbb{R}^d)$ it holds $|\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} f(x) g(x-y) h(y) \, dxdy| \leqslant \|f\|_p \|g\|_q \|h\|_r$.
(vii) *Application of Young:* Let $1 \leqslant \frac{1}{p} + \frac{1}{q} \leqslant 2$, $f \in L^p(\mathbb{R}^d)$, $g \in L^q(\mathbb{R}^d)$, $1 + \frac{1}{r'} = \frac{1}{p} + \frac{1}{q}$. Then $f * g = \int f(y) g(\cdot - y) dy$ fulfills $\|f * g\|_{r'} \leqslant \|f\|_p \|g\|_q$.
(viii) *Riesz-Thorin interpolation:* Suppose there are exponents $1 \leqslant p_0, q_0, p_1, q_1 \leqslant \infty$ and $T : L^{p_0} \cap L^{p_1} \to L^{q_0} \cap L^{q_1}$ is linear. If $\|T\|_{p_0 \to q_0}, \|T\|_{p_1 \to q_1} < \infty$ then for any $t \in [0,1]$, $\|T\|_{p_t \to q_t} \leqslant \|T\|_{p_0 \to q_0}^{1-t} \|T\|_{p_1 \to q_1}^t$, where $\frac{1}{p_t} = \frac{1-t}{p_0} + \frac{t}{p_1}$ and $\frac{1}{q_t} = \frac{1-t}{q_0} + \frac{t}{q_1}$.
(ix) *Hausdorff-Young:* For $\frac{1}{p} + \frac{1}{q} = 1$, $p \in [1,2]$: $\|\hat{f}\|_q \leqslant \|f\|_p$ (this extends the fourier transform to a bounded map from $L^p(\mathbb{R}^d)$ to $L^q(\mathbb{R}^d)$.

The Sobolev space H^1. We say $f \in L^2(\Omega)$ belongs to $H^1(\Omega)$, if there is a function $g = (g_1, \dots, g_d) \in L^2(\Omega \to \mathbb{C}^d)$ s.t. g is the *distributional/weak gradient* of f, i.e. if

$$\int_\Omega f \frac{\partial \phi}{\partial x_j} = -\int g_j \phi \qquad \forall \phi \in C_0^\infty(\Omega)$$

Then we write $g = \nabla f$ (unique).

(i) If $f \in C^1(\Omega) \cap L^2(\Omega)$ then $f \in H^1$ and the usual gradient coincides with the distributional one.
(ii) $H^1(\Omega)$ is a Hilbert space with $\langle f, g\rangle_{H^1} := \langle f, g\rangle + \langle \nabla f, \nabla g\rangle$.
(iii) $\|\nabla f\|_2 \leqslant \|f\|_{H^1}$, i.e. ∇ is a bounded linear operator from $H^1(\Omega)$ to $L^2(\Omega)$.
(iv) *Leibniz rule:* For $f \in H^1(\Omega)$, $\psi \in C^\infty$, then $f\psi \in H^1(\Omega)$ and $\nabla(f\psi) = f\nabla\psi + \psi\nabla f$.
(v) *Chain rule:* Let $G : \mathbb{C}^N \to \mathbb{C}$ be differentiable with bounded and continuous derivatives and $u = (u_1, \dots, u_N)$ with $u_i \in H^1(\Omega)$, then $K := G \circ u \in H^1(\Omega)$ with the extra assumption that if $|\Omega| = \infty$, then $G(0) = 0$. Furthermore $\partial_j K = \sum_k \partial_k G\, \partial_j u_k$.
(vi) *Integration by parts:* For $\Omega = \mathbb{R}^d$, $u, v \in H^1(\mathbb{R}^d)$ it holds $\int_{\mathbb{R}^d} u \frac{\partial v}{\partial x_j} = -\int_{\mathbb{R}^d} \frac{\partial u}{\partial x_j} v$ for $j = 1, \dots, d$.
(vii) **Fourier characterization:** Let $f \in L^2(\mathbb{R}^d)$, then $f \in H^1(\mathbb{R}^d) \Leftrightarrow$ the function $k \mapsto |k|\hat{f}(k)$ is in $L^2(\mathbb{R}^d)$. In this case $\widehat{\nabla f}(k) = 2\pi i k \hat{f}(k)$, $\|f\|_{H^1}^2 = \int (1 + 4\pi^2|k|^2)|\hat{f}(k)|^2 dk$.

Sobolev inequalities.

(i) $\forall f \in H^1(\mathbb{R}^d), d \geqslant 3$: $\|f\|_{\frac{2d}{d-2}} \leqslant S_d \|\nabla f\|_2$
(ii) $\forall f \in H^1(\mathbb{R})$: $\|f\|_\infty^2 \leqslant \frac{1}{2}\|f\|_{H^1}^2$ and f is Hölder-continuous with exponent $1/2$, i.e. $|f(x) - f(y)| \leqslant \|f'\|_2\, |x-y|^{1/2}$ in particular $H^1(\mathbb{R}) \subset C(\mathbb{R})$.
(iii) $\forall f \in H^1(\mathbb{R}^2), q \in [2, \infty)$: $\|f\|_q \leqslant C_q \|f\|_{H^1}$.

Variational principle

Domination of the kinetic energy. Let $V_- \in L^{d/2} + L^\infty$ for $d \geqslant 3$, $V_- \in L^{1+\varepsilon} + L^\infty$ for $d = 2$, $V_- \in L^1 + L^\infty$ for $d = 1$, then $\exists\, C$ depending only on V s.t. $\mathcal{E}(\psi) \geqslant -C\|\psi\|^2$, i.e. $E_0 > -\infty$, and $\exists\, D$ s.t.

$$\int |\nabla\psi|^2 \leqslant 2\mathcal{E}(\psi) + D\|\psi\|^2$$

Weak convergence. A sequence $\{f_k\} \subset L^p$ converges weakly to $f \in L^p$, $f_k \rightharpoonup f$, if

$$l(f_k) \to l(f) \quad \forall l \in (L^p)^*$$

i.e. $f_n \rightharpoonup f \Leftrightarrow \forall g \in L^q : \int f_n g \to \int fg$ (q dual to p). Norm conv. implies weak conv. ($|l(f_k) - l(f)| \leqslant \|l\|\|f_k - f\|$) but not the other way around (osc. to death, walking out to inf., scaling). Properties:

(i) Weak convergence seperates: $f_k \rightharpoonup f$, $f_k \rightharpoonup g \Rightarrow f = g$.
(ii) The norm may drop under the weak limit, i.e. if $f_k \rightharpoonup f$, then $\|f\|_p \leqslant \liminf_k \|f_k\|_p$.
(iii) *Uniform boundedness principle:* If $l(\psi_j)$ is a bounded sequence for any bounded linear functional l (especially if ψ_j is weakly convergent), then $\sup_j \|\psi_j\| < \infty$.
(iv) *Mazur theorem:* If $f_j \in L^p$ converges weakly to $f \in L^p$, then there is a convex combination of f_j that converges strongly to f, i.e. $\exists\, c_{jk} \geqslant 0$, $1 \leqslant k \leqslant j$ with $\sum_{k=1}^j c_{jk}$ s.t. $F_j := \sum_{k=1}^j c_{jk} f_k \to f$.

Variational characterization of the L^2-norm. Since $(L^2)^* = L^2$ and $\|f\|_2 = \|f^*\| = \sup_{g \in L^2}\{|f^*(g)|/\|g\|_2\}$ for any $f \in L^2$ and its dual $f^* \in (L^2)^*$, we have

$$\begin{aligned}\|f\|_2 &= \sup\{|\langle f, g\rangle| : g \in L^2, \|g\|_2 = 1\} \\ &= \sup\{\langle f, \phi\rangle| : \phi \in C_0^\infty, \|\phi\|_2 = 1\}\end{aligned}$$

Where the last equality follows from the fact that C_0^∞ is dense in L^2, i.e. any $g \in L^2$ can be approximated arbitrary well.

Alaoglu-type theorem. Let f_j be a bounded sequence in L^p (or in a separable Hilbert space), i.e. $\sup_j \|f_j\|_p < \infty$, then f_j has a weakly convergent subsequence.

Existence of the minimizer. Assume $V : \mathbb{R}^d \to \mathbb{R}$ satisfies the same conditions as V_- in the theorem about domination of the kinetic energy and assume that V vanishes at infinity, i.e. $|\{x : |V(x)| > a\}| < \infty\ \forall a > 0$. From above we know, that $E_0 > -\infty$ and one can show that $E_0 \leqslant 0$. Now we assume $E_0 < 0$. Then $\exists\, \psi \in H^1, \|\psi\|_2 = 1$ s.t.

$$\mathcal{E}(\psi) = E_0$$

Moreover ψ satisfies $-\Delta\psi + V\psi = E_0\psi$ in a weak sense, i.e. by testing against any $\phi \in C_0^\infty$:

$$\int \overline{\psi}(-\Delta\phi) + \int V\overline{\psi}\phi = E_0 \int \overline{\psi}\phi$$

Sketch of proof:

(i) Choose a min. seq. $\{\psi_n\} \subset H^1$, $\mathcal{E}(\psi_n) \to E_0$, $\|\psi_n\|_2 = 1$.
(ii) By the theorem about domination of the kinetic energy: $\|\nabla\psi_n\|^2 \leqslant 2\mathcal{E}(\psi_n) + D\|\psi_n\|^2 = 2\mathcal{E}(\psi_n) + D$. It follows that $\sup_n \|\psi_n\|_{H^1} < \infty$.
(iii) Since H^1 is seperable Hilbert space, by the Alaoglu-type theorem, there is a weakly convergent subsequence $\psi_j := \psi_{n_j} \rightharpoonup \psi \in H^1$.
(iv) **Claim 1:** $\int |\nabla\psi|^2 \leqslant \liminf_j \int |\nabla\psi_j|^2$.
(Use the variational characterization of the L^2 norm of $\nabla\psi$ and calculate $|\langle\nabla\psi, \phi\rangle| = |\langle\psi, \nabla\phi\rangle| = \lim_j |\langle\psi_j, \nabla\phi\rangle|$, since $\psi_n \rightharpoonup \psi$ in L^2 as well b/c H^1 is dense in L^2. From $\sup_n(\liminf_j a_{nj}) \leqslant \liminf_j(\sup_n a_{nj})$ follows the claim.)
(v) **Claim 2:** $\int V|\psi|^2 = \lim_j \int V|\psi_j|^2$.
(We want to use Rellich-Kondrashev. For this purpose we perform the following steps: (i) Define $V^\delta = V\, \mathbb{1}_{\{x : |V(x)| \leqslant 1/\delta\}}$ where δ is chosen small enough s.t. the L^∞-part of V gets absorbed when computing $V - V^\delta$. (ii) By monotone conv. theorem and $V_\delta(x) \to V(x)$ as $\delta \to 0$ we get $\|V - V^\delta\|_{d/2} \to 0$. (iii) Since $\int (V - V^\delta)|\psi_j|^2 \leqslant \|V - V^\delta\|_{d/2}\|\psi_j\|_{2d/d-2} \leqslant C\|V - V^\delta\|_{d/2}\|\psi_j\|_{H^1}$ (by Sobolev) and $\sup\|\psi_j\|_{H^1} < \infty$, the integral $\int V|\psi_j|^2$ can be replaced by $\lim_{\delta\to 0}\int V^\delta|\psi_j|^2$ (uniformly in j and the same holds for ψ, so we can interchange limits and work from know on with V^δ). (iv) For $\varepsilon > 0$ set $A_\varepsilon := \{x : |V^\delta(x)| > \varepsilon\}$. Since V vanishes at ∞ we have $|A_\varepsilon| < \infty$, so A_ε will be the set for Rellich-Kondrashev. Furthermore $\int V^\delta|\psi_j|^2 = \int_{A_\varepsilon} V^\delta|\psi_j|^2 + \int_{A_\varepsilon^c} \dots$ where the second integral is $\leqslant \varepsilon$ uniformly in j (the same holds for ψ so we can work with $\int_{A_\varepsilon}$). (v) In order to apply RK, we calculate $|\int_{A_\varepsilon} V^\delta(|\psi_j|^2 - |\psi|^2)| \leqslant \frac{1}{\delta}\int_{A_\varepsilon} ||\psi_j|^2 - |\psi|^2|$. Using $|\psi_j|^2 - |\psi|^2 = (|\psi_j| - |\psi|)(|\psi_j| + |\psi|)$ we get $|\dots| \leqslant \frac{1}{\delta}(\int_{A_\varepsilon}|\psi_j - \psi|^2)^{1/2}\int 2(|\psi_j|^2 + |\psi|^2) = \frac{4}{\delta}(\int_{A_\varepsilon}(\psi_j - \psi)^2)^{1/2}$ and by RK the last integral converges to zero.)
(vi) **Claim 3:** $\|\psi\|_2 = 1$.
(By claim 1 and 2: $E_0 = \lim_j \mathcal{E}(\psi_j) \geqslant \mathcal{E}(\psi) \geqslant E_0\|\psi\|_2^2$. So $\|\psi\| \geqslant 1$, b/c $E_0 < 0$. But also $\|\psi\|_2 \leqslant \liminf_j \|\psi_j\|_2 = 1$.)

(vii) ψ **is a ground state**, i.e. $\mathcal{E}(\psi) = E_0$, b/c from the claims above follows: $\mathcal{E}(\psi) \leqslant \liminf_j \mathcal{E}(\psi_j) = E_0$ and clearly $\mathcal{E}(\psi) \geqslant E_0$ always.

(viii) Let $\phi \in C_0^\infty$ and set $\psi^\varepsilon = \psi + \varepsilon\phi$ and $R(\varepsilon) := \mathcal{E}(\psi^\varepsilon)/\|\psi^\varepsilon\|^2$ that is a ratio of two quadratic polynomials in ε with $R(0) = E_0$. Thus R is differentiable in a neighbourhood of 0 and attains its minimum there, so $0 = R'(0)$. This leads to $\Re \int \bar{\psi}(-\Delta\phi + V\phi - E_0\phi) = 0$ after performing an int. by parts in H^1. We get the imaginary part of the same expression by replacing ϕ by $i\phi$. Thus the equality holds for the expression alone.

Rellich-Kondrashev. Let $B \subset R^d$ with $|B| < \infty$ and $f_n \rightharpoonup f$ in $H^1(\mathbb{R}^d)$. Then for any $q \in [1, \frac{2d}{d-2}]$ if $d \geqslant 3$, $q \in [1, \infty)$ if $d = 2$ or $q \in [1, \infty]$ if $d = 1$, we have

$$\lim_{n\to\infty} \int_B |f_n - f|^q = 0$$

There are two implications (the second one is more an equivalent formulation of Rellich-Kondrashev):

(i) **Corollary 1:** If $f_n \rightharpoonup f$ in $H^1(\mathbb{R}^d)$, then there is subsequence $\{f_{n_j}\}$ s.t. $\lim_{j\to\infty} f_{n_j}(x) = f(x)$ for a.e. $x \in \mathbb{R}^d$.

(ii) **Corollary 2:** Any bounded sequence in $H^1(\mathbb{R}^d)$ has a convergent subsequence in $L^q(B)$, where B and q are as above.

(Since $\|f_n\|_{L^q(B)} \leqslant C(B,q)\|f_n\|_{2d/d-2} \leqslant C'\|f_n\|_{H^1}$ and $\sup_n \|f_n\|_{H^1} < \infty$, f_n is bounded in $L^q(B)$. By the Banach-Alaoglue-type theorem, f_n has an H^1-weakly convergent subsequence and by RK, this subsequence converges strongly in $L^q(B)$.)

Sketch of proof of Rellich-Kondrashev: Let $d \geqslant 3$, $q = 2$.

(i) *Smoothing:* Fix $\phi \in C_0^\infty$, $\int \phi = 1$ and define for $m > 0$, $\phi_m := m^d\phi(my)$, then $\int \phi_m = 1$ and $\int |\phi_m(y)||y|dy = \frac{1}{m}\int |\phi(y)||y|dy$

(ii) *Splitting:* We use that $\|f * \phi_m - f\|_2 \to 0$ as $m \to \infty$ and split $\|f_n - f\|_{L^2(B)}$ in the 3 terms $\|f_n - f_n * \phi_m\|_{L^2(B)}$, $\|f_n * \phi_m - f * \phi_m\|_{L^2(B)}$ and $\|f * \phi_m - f\|_{L^2(B)}$.

(iii) *Uniformity of the first limit:* For any $f \in H^1$ we have $\int |f(x+h) - f(x)|^2 dx = \int |e^{2\pi ik\cdot h} - 1|^2 |\hat{f}(k)|^2 dk \leqslant 4\pi^2|h|^2 \int |k|^2|\hat{f}(k)|^2 dk = |h|^2\|\nabla f\|_2^2$. With ϕ from (i), we have $\|f * \phi - f\|_2^2 = \|\int [f(\cdot - y) - f(\cdot)]\phi(y)dy\|_2^2 \leqslant \int |\phi(y)|\,\|f(\cdot - y) - f(\cdot)\|_2^2 dy$ by gen. Minkowski. Using the first result, this gives $\|f * \phi - f\|_2 \leqslant \|\nabla f\|_2 \int |\phi(y)||y|dy$. Applying this to f_n and ϕ_m and using that f_n is uniformly bounded in H^1, we get

$$\|f_n * \phi_m - f_n\|_2 \leqslant \|\nabla f_n\| \int |\phi_m(y)||y|dy \leqslant \frac{C}{m}$$

and the constant C is indep. of n, i.e. for $m \to \infty$ is uniform.

(iv) *Middle term:* $|f_n * \phi_m(x)| \leqslant \|f_n\|_2\|\phi_m\|_2 \leqslant C\|\phi_m\|_2$ and $|f_n * \phi_m(x) - f * \phi_m(x)| \leqslant \|f_n - f\|_2\|\phi_m\|_2 \to 0$ as $n \to \infty$. Thus, by dominated convergence (b/c $|B| < \infty$) we get $\|f_n * \phi_m - f * \phi_m\|_{L^2(B)} \to 0$ as $n \to \infty$ for any fixed m.

(v) *Finally* performing an $\epsilon/3$-argument to the terms, we proved RK for $q = 2$.

(vi) $1 \leqslant q < 2$: $\|f_n - f\|_{L^q(B)} \leqslant C(B,q)\|f_n - f\|_{L^2(B)} \to 0$.

(vii) $2 \leqslant q < \frac{2d}{d-2}$: $\|f_n - f\|_{L^q(B)} \leqslant \|f_n - f\|_2^\theta \|f_n - f\|_{2d/d-2}^{1-\theta}$
$\leqslant \|f_n - f\|_2 (C\|\nabla(f_n - f)\|_2)^{1-\theta} \leqslant C\|f_n - f\|_2^\theta \to 0$.

Distributions. We use the space $C_0^\infty(\Omega)$ (where $\Omega \subset \mathbb{R}^d$) as the space of *test functions* and denote it by $\mathcal{D}(\Omega)$, if it is equipped with the following notion of convergence: $\phi_n \to \phi \Leftrightarrow \exists\, K \subset \Omega$ compact s.t. $\operatorname{supp}(\phi_n - \phi) \subset K$ and for any multiindex α, $D^\alpha\phi_n \to D^\alpha\phi$ unif. on K. *Distributions* $T \in \mathcal{D}'(\Omega)$ are the bounded linear functionals on $\mathcal{D}(\Omega)$ equipped with $T_n \to T :\Leftrightarrow T_n(\phi) \to T(\phi)$, $\forall \phi \in \mathcal{D}(\Omega)$.

(i) *Examples for distributions:* $f \in L^1_{loc}$, then $T_f(\phi) := \int f\phi$; μ regular Borel measure, then $T_\mu(\phi) = \int \phi\, d\mu$; $x \in \mathbb{R}^d$, then $\delta_x(\phi) := \phi(x)$.

(ii) *Derivative of distributions:* For $T \in \mathcal{D}'(\Omega)$ and any multiindex α, $D^\alpha T(\phi) := (-1)^{|\alpha|}T(D^\alpha\phi)$ defines a distribution $D^\alpha T \in \mathcal{D}'(\Omega)$. It is easy to check, that if $T_n \to T$, then $D^\alpha T_n \to D^\alpha T$.

(iii) If $f \in C^\infty$, then $D^\alpha T_f = T_{D^\alpha f}$.

(iv) If $T \in \mathcal{D}'(\Omega)$ s.t. $T^{(1)}$ is a continuous function, then there is $f \in C^1$ s.t. $T = T_f$.

(v) *Fundamental theorem of calculus:* For a function $f \in W^{1,1}_{loc} = \{f \in L^1_{loc} | \nabla f \in L^1_{loc}\}$, we have $f(x+y) - f(x) = \int_0^1 y \cdot \nabla f(x+ty)dt$, $\forall y$ and a.e. x.

(vi) *Integration by parts:* For $v \in L^1_{loc}$, $v(x) \in \mathbb{R}$, $\nabla v \in L^1_{loc}$, $u\nabla v \in L^1$ for any $u \in L^1$, then $-\int u\Delta v = \int \nabla u \nabla v$.

(vii) If Ω is connected and $\nabla T = 0$, then $T = T_{const}$.

(viii) If $\psi \in C^\infty$, $T \in \mathcal{D}'(\Omega)$, then $\psi T(\phi) := T(\psi\phi)$ defines a distribution, i.e. $\psi T \in \mathcal{D}'(\Omega)$.

(ix) *Convolution:* For $j \in C_0^\infty$, we can extend the usual convolution to $\mathcal{D}'(\Omega)$ by $(j * T)(\phi) := T(\int j(y)\phi(\cdot + y)dy)$ and this distribution is given by a function: There is $t \in C^\infty$ s.t. $(j * T)(\phi) = \int t(y)\,\phi(y)\,dy$. Moreover, if $j_\varepsilon := \varepsilon^{-d}j(x/\varepsilon)$, then $j_\varepsilon * T \to T$ in $\mathcal{D}'(\Omega)$.

(x) If $\{\psi_j\}_1^N$ is an ONS in $L^2(\Omega)$, $T \in \mathcal{D}'(\Omega)$ s.t. $T(\phi) = 0$ $\forall \phi$ with $\langle \phi, \psi_j \rangle = 0\ \forall j$, then $\exists\, c_j$ s.t. $T = \sum_j c_j\psi_j$.

(xi) Suppose $T(\phi) = 0$ for any $\phi \in \mathcal{D}(\Omega)$ with supp $\phi \subset \Omega\backslash\{0\}$. Then there is $K \in \mathbb{N}$ and c_j s.t. $T = \sum_{j=0}^K c_j\delta_0^{(j)}$.

(xii) A distribution T is called positive, if $T(\phi) \geqslant 0$ for all $\phi \geqslant 0$. Positive distributions are regular Borel measures.

Excited states. Let $H = -\Delta + V$ where V satisfies the same conditions as in the theorem on the domination of the kin. energy. Let E_0 be the ground state energy and ψ_0 (one of) the groundstate(s). Assume $E_0 \leqslant \ldots \leqslant E_{k-1}$ and $\psi_0, \ldots, \psi_{k-1}$ are known, then $E_k := \inf\{\mathcal{E}(\psi) | \psi \in H^1(\mathbb{R}^d), \|\psi\|_2 = 1, \langle\psi, \psi_j\rangle = 0, j = 0, \ldots, k-1\}$.

(i) Assume the first k eigenstates exist and $E_k < 0$, then the $(k+1)$th eigenstate ψ_k, i.e. the minimizer for E_k, also exists and satisfies the Schrödinger eq. $H\psi_k = E_k\psi_k$ in a weak sense. Thus the recursion from above can only stop for $E_k = 0$.

(ii) If $E_k < 0$, then the multiplicity is finite.

(iii) The sequence $E_0 \leqslant E_1 \leqslant \ldots$ cannot accumulate at any negative number.

(iv) The ψ_k may not be unique, but the eigenspace is.

(v) The eigenfunctions can be chosen real.

Properties of eigenfunctions. We assume the conditions on V as above and $E_0 < 0$, then

(i) The ground state is unique.
(ii) The ground state can be chosen strictly positive.
(iii) The positivity of an eigenfunction characterizes the ground state, i.e. if $H\psi = E\psi$ for some $\psi \in H^1$ with $\psi \geqslant 0$, then $E = E_0$ and ψ is the ground state.
(iv) If V is spherically symmetric, i.e. $V(x) = V(|x|)$, so is the ground state.
(v) If $(-\Delta + V)\psi = E\psi$ holds on a ball $B \subset \mathbb{R}^d$ in the sense of distributions and $V \in C^k(B)$, then $\psi \in C^{k+2}(B)$, i.e. ψ is even a strong solution.

Lemma. If $f \in H^1$, then $|f| \in H^1$ and

$$\int |\nabla |f||^2 \leqslant \int |\nabla f|^2$$

actually it holds even pointwise that $|\nabla|f|| \leqslant |\nabla f|$. Moreover, if $|f(x)| > 0$, then equality holds only if $\exists\ \lambda \in \mathbb{C}$ with $|\lambda| = 1$ and $f(x) = \lambda|f(x)|$.

Many body quantum systems

Marginal density of the i-th particle. It is the probability distribution of the i-th particle that is given by

$$\rho^i_\psi(x) = \int |\psi(\ldots, x_{i-1}, x, x_{i+1}, \ldots)|^2\, dx_1 \ldots \widehat{dx_i} \ldots$$

One-particle density function. The particle density in the state ψ is given by $\rho_\psi(x) := \sum_{i=1}^N \rho^i_\psi(x)$. We have

$$\int_{\mathbb{R}^d} \rho_\psi = \sum_{i=1}^N \int \rho^i_\psi = \sum_{i=1}^N 1 = N$$

(If ψ is symmetric or antisymmetric, we have $\rho^i_\psi = \rho^1_\psi$ for all i and thus $\rho_\psi = N\rho^1_\psi$.)

Density matrix. For a normalized $\psi \in L^2(\mathbb{R}^{Nd})$ we define its *density matrix* as the orthogonal projection onto the subspace spanned by ψ, i.e. $(\Gamma_\psi \phi)(\boldsymbol{x}) := \langle \psi, \phi\rangle \psi(\boldsymbol{x})$. It has the kernel $\Gamma_\psi(\boldsymbol{x}, \boldsymbol{x}') = \psi(\boldsymbol{x})\overline{\psi}(\boldsymbol{x}')$.

One-particle density matrix. Given a density matrix Γ_ψ of an N-particle state ψ, we define a one-particle operator $\gamma^{(1)}_\psi : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$ with kernel $\gamma^{(1)}_\psi(x, x') := \sum_i \int \Gamma_\psi(\ldots, x_{i-1}, x, \ldots; \ldots, x_{i-1}, x', \ldots) \ldots dx_{i-1}dx_{i+1} \ldots$ (then $\gamma^{(1)}_\psi(x,x) = \rho_\psi(x)$ is the one-p. density from above).

Simplest bosonic state. If $\{f_j\} \subset L^2(\mathbb{R}^d)$, then the function $f_J := f_{j_1} \otimes \cdots \otimes f_{j_N} \in L^2(\mathbb{R}^{Nd}) = \bigotimes_1^N L^2(\mathbb{R}^d)$ (where $J = (j_1, \ldots, j_N)$) is not symmetric, but after applying the *symmetrization* $\mathcal{S} : \bigotimes L^2(\mathbb{R}^d) \to \bigotimes^s L^2(\mathbb{R}^d)$, $\psi \mapsto \sum_{\pi \in S_N} \psi(x_{\pi(1)}, \ldots)$, the function $f_{\otimes J} := \mathcal{S}(\bigotimes_{l=1}^N f_{j_l})$ describes a simple bosonic state (where $J = \{j_1, \ldots, j_N\}$). The normalized operator $\frac{1}{N!}\mathcal{S}$ is an orthogonal projection. If $\{f_j\}$ is an ONB in $\mathcal{H}$, then $\{f_J | J = (j_1, \ldots, j_N)\}$ is an ONB in $\bigotimes H$ and $\{\frac{1}{N!} f_{\otimes J} | J = \{j_1, \ldots, j_N\}\}$ forms an ONB in $\bigotimes^s \mathcal{H}$.

Simplest fermionic state. If $\{f_j\} \subset L^2(\mathbb{R}^d)$, the *antisymmetrized tensor product* or *Slater determinant* is def. by $f_1 \wedge \ldots \wedge f_N(x_1, \ldots, x_N) = \frac{1}{\sqrt{N!}} \det(f_i(x_j))$. It can also be defined using the *total antisymmetrization* $\mathcal{A}$ that is given by $(\mathcal{A}\psi)(x_1, \ldots, x_N) = \sum_{\pi \in S_N} sgn(\pi)\psi(x_{\pi(1)}, \ldots)$. Then $f_1 \wedge \cdots \wedge f_N = \frac{1}{\sqrt{N!}} \mathcal{A}(f_1 \otimes \cdots \otimes f_N)$.

Many spins. If the number of spins q is bigger than the number of particles, $q \geqslant N$, then the fermionic character can be completeley forgotten, i.e. the following holds: If $\phi(\boldsymbol{x})$ is an arbitrary function in $L^2(\mathbb{R}^{Nd})$ depending only on the space variables, then we can trivially extend this function to be an antisymmetric function as $\psi((x_1, \sigma_1), \ldots) = \frac{1}{\sqrt{N!}} \mathcal{A}(\phi(\boldsymbol{x})) \prod_1^N \delta(\sigma_j = j))$, i.e. even if ϕ is a symmetric function depending only on space, we can construct an antisymmetric one (in the spin variables) out of it. This is useful because of the properties

(i) $\|\psi\| = \|\phi\|$
(ii) For H being indep. of spin and invariant under perm. of space variables, we have $\langle \phi, H\phi\rangle = \langle \psi, (H \otimes I)\psi\rangle$.

Therefore $E^f_0(q \geqslant N) = E_0$.

The ground state is bosonic. For $H = H_0 + W$, where $W(\boldsymbol{x}) = \sum_{i<j} U(x_i - x_j)$ with $U(x) = (-x)$ and $H_0 = \sum_i h_i$ where $h_i = -\Delta_i + V(x_i)$. Suppose $\mathcal{E}(\psi)$ is bounded from below, i.e. $E_0 > -\infty$, then $E_0 = E^b_0$.

Non-interacting bosons. Let $H = H_0$ and assume that the groundstate energy of the one-particle problem described by h is finite. Then $E_0 = Ne_0$. Moreover if the ground state f_0 of h exists, then $\psi_0 = f_0 \otimes \cdots \otimes f_0$ is the unique ground state of H_0.

Bounded operators. Let $\mathcal{H}$ be a seperable Hilbert space, $A : \mathcal{H} \to \mathcal{H}$ a bounded linear operator.

(i) The adjoint of A, A^*, is def. by $\langle x, Ay\rangle = \langle A^*x, y\rangle$.
(ii) A is called self-adjoint, if $A = A^*$ and A is called unitary, if $A^*A = AA^* = id$.
(iii) $A = A^* \Leftrightarrow \langle x, Ax\rangle \in \mathbb{R}\ \forall x \in \mathcal{H}$.
(iv) $\rho(A) := \{z \in \mathbb{C} | (z-A)^{-1}$exists and is bounded$\}$ is called the resolvent set of A ($\rho(A) \subset \mathbb{C}$ open).
(v) $\sigma(A) = \mathbb{C}\backslash\rho(A)$ is called spectrum of A ($\sigma(A) \neq \emptyset$).
(vi) Eigenvalues of A are elements of the spectrum.
(vii) $\sigma = \sigma_p \cup \sigma_c$ where $\sigma_p = \{$ev's$\}$ is the point spectrum and $\sigma_c = \sigma\backslash\sigma_p$ is the continuous spectrum.
(viii) A *compact operator* has the following equivalent properties: (1) A maps bounded sets to compact ones. (2) If $\{x_n\} \subset \mathcal{H}$ is bounded, then $\{Ax_n\}$ has a convergent subsequence. (3) A can be approximated in the operator norm by finite rank operators.
(ix) The typical example of a compact operator on function spaces has an integral kernel: $Af(x) = \int a(x,y)f(y)dy$.
(x) The compact operators form an ideal in the set of bounded operators, i.e. if A is compact and B bounded, then AB and BA are compact.
(xi) If A is compact, then $\sigma(A)\backslash\{0\}$ consists of eigenvalues with finite multiplicity and the eigenvalues may accumulate only at 0.
(xii) *Spectral theorem:* For a compact and s.a. operator A, $\exists\{\lambda_j\} \subset \mathbb{R}$ and $\exists!$ ONB $\{v_j\}$ s.t. $Ax = \sum_{j=1}^\infty \lambda_j \langle v_j, x\rangle v_j$.