11. Examples and applications

11.1. 1D step-potentials

* Suppose $V \in C^{(1)}(\mathbb{R}) \cap L^\infty(\mathbb{R})$ is monotone decreasing. Then a classical particle with mass $= 1$ moving under the influence of the potential V has a trajectory x_t which satisfies $\ddot{x}_t = -V'(x_t) \geq 0$. Hence, its velocity $\dot{x}_t$ can only increase. In particular, if $v_0 := \dot{x}_0 > 0$, then $x_t = x_0 + \int_0^t ds\, \dot{x}_s \geq x_0 + v_0 t$ for all $t \geq 0$. This implies that if the particle starts by moving to the right, it can never be reflected by the potential V: we have $x_t \to +\infty$ as $t \to +\infty$.

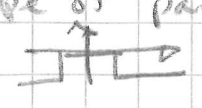
The situation is very different for quantum particles: not only can they be reflected by such potentials, the reflection can even become near certain.

This phenomena is studied from various angles in the paper (link on webpage and copy as an appendix here): Sec. 2-6. in

P. L. Garrido, S. Goldstein, J. Lukkarinen, R. Tumulka: Am. J. Phys. 79 (2011) 1218-1231
Preprint: arxiv.org/abs/0808.0610.

* In Sec. 7-9, with mathematical details given in the Appendices, we also show how to rigorously connect the "Gamow eigenvalues" $z \in \mathbb{C}$ and the associated "eigenvectors" $\psi \notin L^2(\mathbb{R})$ satisfying

$$z\,\psi(x) = -\tfrac{1}{2}\psi''(x) + V(x)\,\psi(x)\,, \quad x \in \mathbb{R},$$

to the "metastable" escape of particles from a potential plateau $V =$  .

11.2. Harmonic oscillator

Consider arbitrary $d \geq 1$ and the potential $V(x) := \frac{\omega^2}{2} x^2$ with $\omega > 0$. Since $V \geq 0$ and $|V(x)| \leq \frac{\omega^2}{2} R^2$ for $|x| \leq R$, we can apply Theorem 10.5. to define a self-adjoint operator H on $L^2(\mathbb{R}^d)$: $H =$ "$(H_0 + V)_{\text{dist}}$".

Suppose then that $\lambda_j \in \mathbb{C}$ and $\psi_j \in C^{(2)}(\mathbb{R})$, $j = 1, \dots, d$, each solve the differential equation

$$-\frac{1}{2} \psi_j''(y) + \frac{\omega^2}{2} y^2 \psi_j(y) = \lambda_j \psi_j(y) \quad \forall y \in \mathbb{R}, \; j = 1, \dots, d.$$

Define $\psi(x) := \prod_{j=1}^{d} \psi_j(x_j)$

$$\Rightarrow -\frac{1}{2} \nabla^2 \psi(x) = -\frac{1}{2} \sum_{i=1}^{d} \partial_{x_i}^2 \left(\prod_{j=1}^{d} \psi_j(x_j) \right)$$

$$= \sum_{i=1}^{d} \prod_{j \neq i} \psi_j(x_j) \cdot \underbrace{\left(-\frac{1}{2} \psi_i''(x_i) \right)}_{= (\lambda_i - \frac{\omega^2}{2} x_i^2) \psi_i(x_i)}$$

$$= \sum_{i=1}^{d} \left(\lambda_i - \frac{\omega^2}{2} x_i^2 \right) \psi(x) = \sum_{i=1}^{d} \lambda_i \cdot \psi(x) - \frac{\omega^2}{2} x^2 \psi(x)$$

$$\Rightarrow -\frac{1}{2} \nabla^2 \psi(x) + \frac{\omega^2}{2} x^2 \psi(x) = \lambda \psi(x) \quad \forall x \in \mathbb{R}^d$$

where $\lambda := \sum_{i=1}^{d} \lambda_i$. If, in addition, each $\psi_j \in L^2(\mathbb{R})$ with $\|\psi_j\| = 1$, then $\int_{\mathbb{R}^d} dx \, |\psi(x)|^2 = \prod_{j=1}^{d} \left(\int dy \, |\psi_j(y)|^2 \right)$ $= 1 \Rightarrow \psi \in L^2(\mathbb{R}^d)$ and $\|\psi\| = 1$. Moreover,

$\psi \in C(\mathbb{R}^d)$ and thus $V\psi \in L^1_{\text{loc}}$ and, if $f \in \mathcal{D}(\mathbb{R}^d)$ with support contained in the box $|x_j| \leq R \; \forall j = 1, \dots, d$,

$$\Rightarrow (\nabla^2 f, \psi) = \sum_{j=1}^{d} \int_{[-R,R]^d} dx \, (\partial_{x_j}^2 f|_x)^* \psi(x) \overset{\text{Fubini \& partial integration}}{=} \sum_{j=1}^{d} \int_{[-R,R]^{d-1}} d\hat{x}$$

$$\times \Big[\underbrace{\Big/_{-R}^{R} \partial_{x_j} f^*|_x \, \psi(x)}_{=0} - \int_{-R}^{R} dx_j \, \partial_{x_j} f^*|_x \, \partial_{x_j} \psi(x) \Big] \Big|_{x = \hat{x} + x_j \hat{e}_j}$$

$$= \int_{[-R,R]^d} dx \, f(x)^* \nabla^2 \psi(x) = (f, \nabla^2 \psi)$$

$$\Rightarrow \left(-\tfrac{1}{2}\Delta f, \psi\right) = \left(f, -\tfrac{1}{2}\Delta\psi\right) = \int dx\, f(x)^* \left(\lambda\psi(x) - (V\psi)(x)\right)$$
$$\underset{\psi \in L^2}{=} (f, \lambda\psi) - \int dx\, f(x)^* (V\psi)(x)$$

Hence by Thrm 10.5. then $\psi \in D(H)$ and $H_0\psi = \lambda\psi$.
$\Rightarrow$ ψ is an eigenvector of H with eigenvalue λ.

Proposition: The solutions to equation

$$-\tfrac{1}{2}\psi''(x) + \tfrac{1}{2}\omega^2 x^2 \psi(x) = \lambda\psi(x), \quad x \in \mathbb{R}$$

with $\lambda \in \mathbb{C}$ and $\psi \in C^{(2)}(\mathbb{R}) \cap L^2(\mathbb{R})$ are given by $\lambda = \lambda_n$, $\psi = C\psi_n$, $n = 0, 1, 2, \dots$, $C \in \mathbb{C}$, where

$$\lambda_n := \omega\left(n + \tfrac{1}{2}\right) > 0 \quad \text{and}$$

$$\psi_n(x) := \frac{1}{\sqrt{n!\,2^n}} \left(\frac{\omega}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\omega}{2}x^2} H_n(\omega^{\frac{1}{2}} x), \quad x \in \mathbb{R},$$

and H_n denotes the n:th Hermite polynomial satisfying

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}.$$

In addition, $\|\psi_n\|_{L^2} = 1$, and $(\psi_n)_{n \in \mathbb{N}_0}$ forms an ONB for $L^2(\mathbb{R})$.

Proof: Parts of it can be found in any QM textbook. For mathematical details see e.g. Teschl Sec. 9.2. Completeness of $(H_n)_n$ is outlined e.g. on p. 121, problem 7, of Reed & Simon II. $\square$

* Since (ψ_n) forms an ONB for $L^2(\mathbb{R})$, by the Proposition on p. 24, the functions $\psi_{\bar{n}} := \prod_{i=1}^{d} \psi_{n_i}(x_i)$, $\bar{n} \in \mathbb{N}_0^d$,

form an ONB for $\bigotimes_{i=1}^{d} L^2(\mathbb{R}) \cong L^2(\mathbb{R}^d)$. Defining $\lambda_{\bar{n}} := \sum_{i=1}^{d} \lambda_{n_i} = \omega\left(\frac{d}{2} + \sum_{i=1}^{d} n_i\right) \in \mathbb{R}$, one can rely

on uniqueness of the spectral representation to conclude that $\sigma(H) = \bigcup_{\bar{n} \in \mathbb{N}_0^d} \{\lambda_{\bar{n}}\}$, and $\inf \sigma(H) = \frac{\omega d}{2} > 0$, non-degenerate eigenv.

11.3. Example: Hydrogen atom

Consider $d=3$ and $V(x) = -\frac{\gamma}{|x|}$, for $\gamma > 0$.

(For a specific choice of constants this corresponds to movement of electron around the proton in a hydrogen atom. The proton is assumed to be at $x=0$, which is also an approximation: proton is treated classically, and we are in the "comoving" coordinate system. ($x = \underline{X}_{\text{electron}} - \underline{X}_{\text{proton}}$, $\underline{X} \in \mathbb{R}^3$ denoting positions in the "laboratory frame".) Then $\gamma = \alpha_{\text{fine}} \approx 7.3 \cdot 10^{-3}$.)

Here $V = V_{\leq} + V_{>}$ with $V_{\leq}(x) := -\frac{\gamma}{|x|} \mathbb{1}(|x| \leq 1)$

and $V_{>}(x) := -\frac{\gamma}{|x|} \mathbb{1}(|x| > 1)$. Now $|V_{>}(x)| \leq \gamma < \infty$

and $\int_{\mathbb{R}^3} dx\, |V_{\leq}(x)|^2 = \int_0^\infty dr\, r^2 \frac{\gamma^2}{r^2} \mathbb{1}(r \leq 1) \cdot 4\pi$

$= 4\pi \gamma^2 \int_0^1 dr < \infty$. $\Rightarrow V_{>} \in L^\infty$, $V_{\leq} \in L^2$.

Thus by Kato-Rellich theorem $H_c = H_0 + V$ is self-adjoint on $D(H_0)$.

The following results are computed in most QM textbooks and mathematically derived in Teschl's book, chapter 10. (Thrm. 10.9.)

* $\sigma(H_c) = \sigma_p \cup \sigma_0$, were σ_p collects all eigenvalues of H which have a finite eigenspace and $\sigma_0 := \sigma(H_c) \setminus \sigma_p$

Here $\sigma_0 = [0, \infty)$ and $\sigma_p = \bigcup_{n=0}^{\infty} \{+E_n\}$

where $E_n := -\left(\frac{\gamma}{n+1}\right)^2$, $n = 0, 1, \ldots$

$\Rightarrow E_0 < E_1 < \cdots < E_n < \cdots < 0$ and $E_n \nearrow 0$ as $n \to \infty$.
The eigenspace is parametrized by spherical harmonics Y_ℓ^m, $|m| \leq \ell \leq n$ $\Rightarrow$ has $\dim = (n+1)^2$.

11.4. Kato's theorem and Molecular Hamiltonians

Consider a system of N electrons (treated quantum mechanically) moving between M nuclei (at static positions). The charge of any one electron is $-q_e$, $q_e > 0$, and the nucleus with label j is assumed to be at position $\bar{R}_j \in \mathbb{R}^3$ with a charge $+Z_j q_e$, $Z_j \in \mathbb{Z}$, and mass $M_j \times m_e > 0$. (m_e denotes the mass of electron, which in our units is scaled to $m_e = 1$.)

This approximation makes sense for crystalline solids for which the nuclei are always close to their "equilibrium positions" in the crystal structure. Since $M_j \gg 1$ (even for the lightest nucleus, Hydrogen, $M \approx 2000$), typically $\bar{R}_j$ are considered fixed.

The classical electromagnetic interaction potential of such a system is (in our units) $\alpha_{fine} V_C$ where

$$V_c(x; R) := W(x; R) + I(x) + U(R), \quad x \in (\mathbb{R}^3)^N, \; R \in (\mathbb{R}^3)^M$$

with

$$W(x;R) = \text{electron-nucleus interaction potential}$$
$$:= -\sum_{i=1}^{N} \sum_{j=1}^{M} \frac{Z_j}{|\bar{x}_i - \bar{R}_j|}$$

$$I(x) = \text{electron-electron interaction potential}$$
$$:= \sum_{\substack{i',i=1 \\ i'<i}}^{N} \frac{1}{|\bar{x}_{i'} - \bar{x}_i|} \quad (= \text{sum over all e-e-pairs})$$

$$U(R) = \text{nucleus-nucleus potential}$$
$$:= \sum_{\substack{j',j=1 \\ j'<j}}^{M} \frac{Z_{j'} Z_j}{|\bar{R}_{j'} - \bar{R}_j|}$$

The corresponding quantum mechanical model for the movement of the electrons is determined by the Hamiltonian (given $R \in (\mathbb{R}^3)^M$, with $\bar{R}_j \neq \bar{R}_{j'}$, $j' \neq j$)

$$H = H_R := -\frac{1}{2}\sum_{i=1}^{N} \Delta_{\bar{x}_i} + \alpha V_c(x;R), \quad \alpha := \alpha_{\text{fine}}$$
$$= H_0 + \alpha V_c$$

The following result implies that H is a self-adjoint operator, with $D(H) = D(H_0)$, on $L^2((\mathbb{R}^3)^N)$. (Proof left as an Exercise.)

<u>11.4.1. Theorem (Kato)</u> Suppose $N, J \in \mathbb{N}_+$. Assume

$F_j : \mathbb{R}^3 \to \mathbb{R}$, $j = 1, 2, \dots, J$ are Lebesgue measurable and $F_j \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, and suppose that to each $j \in \{1, 2, \dots, J\}$ there corresponds a rotation $O_j \in O(3N)$ (i.e. $O_j \in \mathbb{R}^{3N \times 3N}$ and $O_j^T O_j = 1 = O_j O_j^T$). Let P_3 denote the projection $\mathbb{R}^{3N} \to \mathbb{R}^3$ defined by $(P_3 x)_\nu := x_\nu$ $\forall \nu = 1, 2, 3$.

Set $V_j(x) := F_j(P_3 O_j x)$, $j = 1, \dots, J$, $x \in \mathbb{R}^{3N}$ and define $V(x) := \sum_{j=1}^{J} V_j(x)$, $x \in \mathbb{R}^{3N}$. Then

V is Lebesgue measurable and real-valued, and let V also denote the corresponding self-adjoint multiplication operator.

In this setup, the operator $H = H_0 + \alpha V$ is self-adjoint on $D(H_0)$ for any $\alpha \in \mathbb{R}$. H is also essentially self-adjoint on $\mathcal{D}(\mathbb{R}^{3N})$ and on $\mathcal{S}_{3N}$.

<u>Proof:</u> The preimage of any set $A \subset \mathbb{R}^3$ under the map $x \mapsto P_3 O_j x$ is equal to $O_j^T(A \times \mathbb{R}^{3(N-1)}) \subset \mathbb{R}^{3N}$. In particular, if A is Lebesgue measurable, the preimage is Lebesgue meas. in $\mathbb{R}^{3N}$. Since each F_j is Lebesgue measurable, this implies that every V_j is measurable $\Rightarrow$ V is measurable. Obviously, $V(x) \in \mathbb{R}$ $\forall x$, and thus M_V is a self-adjoint operator on $\mathcal{H} := L^2((\mathbb{R}^3)^N)$. $\Rightarrow$ so is $\alpha V := \alpha M_V$.

Consider then an arbitrary $\psi \in \mathcal{S}_{3N}$ and $F \in L^2(\mathbb{R}^3)$, $O \in O(3N)$. Then

$$I := \int_{\mathbb{R}^{3N}} dx\, |\psi(x)\, F(P_3 O x)|^2$$

$$\overset{y=Ox}{=} \int_{\mathbb{R}^{3N}} dy\, \underbrace{|\det O|}_{=1}\, |\psi(O^T y)\, F(P_3 y)|^2$$

$$\overset{\text{Fubini}}{=} \int_{(\mathbb{R}^3)^{N-1}} dy' \left[\int_{\mathbb{R}^3} dz\, |F(z)|^2\, |\psi(\overbrace{O^T(z,0) + O^T(0,y')}^{\in \mathbb{R}^3 \times (\mathbb{R}^3)^{N-1}})|^2 \right]$$

For $y' \in (\mathbb{R}^3)^{N-1}$ denote $g_{y'}(z) := \psi(O^T(z,0) + O^T(0,y'))$, $z \in \mathbb{R}^3$.

Since $\psi \in \mathcal{S} \Rightarrow g_{y'}(z) = \int_{\mathbb{R}^{3N}} dp\, e^{i2\pi p\cdot O^T(z,y')}\, \hat{\psi}(p)$

$$= \int dp\, e^{i2\pi Op\cdot(z,y')}\, \hat{\psi}(p)$$

$$\Rightarrow -\nabla_z^2 g_{y'}(z) = \int dp\, \underbrace{(2\pi)^2 \sum_{\nu=1}^{3} (Op)_\nu^2\, \hat{\psi}(p)}_{=:\hat{h}(p),\ \hat{h}\in\mathcal{S}}\, e^{i2\pi Op\cdot(z,y')}$$

$$\Rightarrow \|\hat{h}\|_2^2 = \int dp\, |\hat{\psi}(p)|^2 \left(\sum_{\nu=1}^{3} (2\pi Op)_\nu^2\right)^2$$

$$\leq \int dp\, |\hat{\psi}(p)|^2 \Big(\underbrace{\sum_{\nu=1}^{3N} (2\pi Op)_\nu^2}_{=(2\pi)^2|Op|^2 = (2\pi)^2 p^2}\Big)^2$$

$$= \int dp\, |(2\pi p)^2 \hat{\psi}(p)|^2 = \|2H_0\psi\|_2^2 .$$

On the other hand, $\|\hat{h}\|_2^2 = \|h\|_2^2 = \int dx\, |h(x)|^2$

$$\overset{y=Ox}{=} \int dy\, |h(O^T y)|^2 = \int_{(\mathbb{R}^3)^{N-1}} dy' \left[\int_{\mathbb{R}^3} dz\, |-\nabla_z^2 g_{y'}(z)|^2 \right] < \infty$$

$\Rightarrow$ for a.e. y', $\|-\nabla^2 g_{y'}\| < \infty$. Since also

$$\|\psi\|^2 = \int dy\, |\psi(O^T y)|^2 = \int dy' \left[\int dz\, |g_{y'}(z)|^2\right] < \infty .$$

Since $g_{y'} \in \mathcal{S}_3\ \forall y'$ (Exercise), we have $g_{y'} \in D(H_0|_{d=3})$ and

$H_0 g_{y'} = -\frac{1}{2}\nabla^2 g_{y'}$. Thus by Proposition 10.3. $\Rightarrow \forall \varepsilon > 0\ \exists C_\varepsilon > 0$ s.t.

$$|g_{y'}(z)| \leq \varepsilon \|H_0 g_{y'}\|_{L^2(\mathbb{R}^3)} + C_\varepsilon \|g_{y'}\|_{L^2(\mathbb{R}^3)} \quad \forall y', z$$

therefore, $\int dy'\, |g_{y'}(z)|^2 \leq \int dy'\, 2\left(\varepsilon^2 \|H_0 g_{y'}\|^2 + C_\varepsilon^2 \|g_{y'}\|^2\right)$

$$= \frac{\varepsilon^2}{2} \int dy'\, \|-\nabla^2 g_{y'}\|^2 + 2C_\varepsilon^2 \int dy'\, \|g_{y'}\|^2 \leq \frac{\varepsilon^2}{2}\|\hat{h}\|_2^2 + 2C_\varepsilon^2 \|\psi\|^2$$

Thus, by Fubini's theorem,

$$I = \int dz\, |F(z)|^2 \left[\int dy'\, |g_{y'}(z)|^2 \right]$$

$$\leq \|F\|_{L^2}^2 \cdot \left(2\varepsilon^2 \|H_0\psi\|^2 + 2C_\varepsilon^2 \|\psi\|^2 \right) < \infty$$

If $F \in L^\infty(\mathbb{R}^3)$, we similarly obtain

$$\int dx\, |\psi(x) F(P_3 O x)|^2 = \int dy\, |\psi(O^T y) F(P_3 y)|^2$$

$$= \int dy' \left[\underbrace{\int_{\mathbb{R}^3} dz\, |F(z)|^2 \, |\psi(O^T(z,y'))|^2}_{\leq \|F\|_\infty^2 \int dz |\psi(O^T(z,y'))|^2 \ \forall y'} \right]$$

$$\leq \|F\|_\infty^2 \int dy\, |\psi(O^T y)|^2 = \|F\|_\infty^2 \|\psi\|^2 < \infty.$$

This proves that if $\varepsilon > 0$, $\exists C_\varepsilon \geq 0$ s.t. $\forall \psi \in \mathcal{S}_{3N}$, $j = 1, \dots, J$, using $F_j = F_{j,2} + F_{j,\infty}$,

$$\|V_j \psi\| \leq \|F_{j,2}\|_{L^2} \underbrace{\sqrt{2\varepsilon^2 \|H_0\psi\|^2 + 2C_\varepsilon^2 \|\psi\|^2}}_{\sqrt{2a^2+2b^2} \leq \sqrt{4\max(a^2,b^2)} \leq 2(|a|+|b|)} + \|F_{j,\infty}\| \, \|\psi\|$$

$$\leq 2\varepsilon \|F_{j,2}\|_{L^2} \|H_0\psi\| + \left(2C_\varepsilon \|F_{j,2}\|_{L^2} + \|F_{j,\infty}\| \right) \|\psi\|$$

$$\Rightarrow \|V\psi\| \leq \sum_{j=1}^J \|V_j \psi\| \leq \left(2\varepsilon \sum_{j=1}^J \|F_{j,2}\|_{L^2} \right) \cdot \|H_0\psi\|$$

$$+ \sum_{j=1}^J \left(2C_\varepsilon \|F_{j,2}\|_{L^2} + \|F_{j,\infty}\| \right) \cdot \|\psi\|$$

This implies that if $\alpha \in \mathbb{R}$ is given, then $\forall a > 0\ \exists b \geq 0$ s.t.

(*) $\|\alpha V \psi\| \leq a \|H_0\psi\| + b\|\psi\|$ for $\psi \in \mathcal{S}_{3N}$.

Since $\mathcal{S}_{3N}$ is a core for H_0, the Remark on p. 111 implies that then (*) holds for all $\psi \in D(H_0)$.

Therefore, by the Kato-Rellich theorem (10.2.)

$\Rightarrow$ $H = H_0 + \alpha V$ is self-adjoint on $D(H_0)$ and essentially self-adjoint on any core of $D(H_0)$, for instance on $\mathcal{S}_{3N}$ and $\mathcal{D}_{3N}$ $\square$

Remark: This also implies that $D(H_0) \subset D(\alpha V)$. Choose $\psi \in D(H_0)$. Then $\exists \psi_n \in \mathcal{S}$ s.t. $\psi_n(x) \to \psi(x)$ a.e. x and $\psi_n \to \psi$, $H_0\psi_n \to H_0\psi$ in L^2. By Fatou's Lemma $\int dx\, |\alpha V\psi|^2 = \int dx \left(\liminf_{n\to\infty} |\alpha V(x)\psi_n(x)|^2 \right) \leq \liminf_{n\to\infty} \int dx\, |\alpha V \psi_n|^2 \leq (a\|H_0\psi\| + b\|\psi\|)^2 < \infty$. thus then $\psi \in D(M_{\alpha V})$.

11.5. Relativistic Hamiltonians and external magnetic fields

* Suppose the particle has a mass $m > 0$. So far we have taken as the free evolution the one corresponding to classical Newtonian mechanics, $H_0 = \frac{1}{2m}\hat{p}^2 = -\frac{1}{2m}\nabla^2$ on $L^2(\mathbb{R}^3)$.

Other possibilities are encountered in physical applications: For instance,

a) The addition of an external magnetic field, $\bar{B}(x) := \nabla \times \bar{A}(x)$, with $\bar{A} : \mathbb{R}^3 \to \mathbb{R}^3$ denoting the magnetic vector potential, will require using

$$H_{0,\bar{A}} := \frac{1}{2m}\left(-i\nabla - q\,\bar{A}(x)\right)^2, \quad q = \text{charge of particle} \in \mathbb{R}$$

Already the simplest example case, $\bar{B} = \text{const} = \bar{B}_0$ corresponding to $\bar{A}(x) = \frac{1}{2}\bar{x} \times \bar{B}_0$, needs additional machinery to describe $H_{0,\bar{A}}$ as a self-adjoint operator on $L^2(\mathbb{R}^3)$. See, for instance, Theorem X.22 in Reed & Simon II, p. 173.

b) If the free evolution of the particle needs to be described relativisticly, one should replace H_0 by (in units with c = velocity of light $= 1$)

$$H_{rel} := \sqrt{-\nabla^2 + m^2}.$$

This is self-adjoint as $\mathcal{F}^* M_F \mathcal{F}$ where M_F denotes the multiplication operator with $F(2\pi \bar{k})$,

$F(\bar{p}) = \sqrt{\bar{p}^2 + m^2}$. By 6.5.6., H_{rel} is then self-adjoint on $L^2(\mathbb{R}^3)$.

One then has $F(\bar{p}) = m + \frac{1}{2m}\bar{p}^2 + O(\bar{p}^4)$
$\Rightarrow H_{rel} = m\mathbb{1} + H_0 +$ "correction". The corresponding particle densities have a "relativistic" behaviour:

For instance, the scaling limits of Wigner transforms $W^{\varepsilon}_{\psi(\frac{t}{\varepsilon})}$, defined using $\psi(t) := e^{-itH_{rel}}\psi(0)$

and any $\varepsilon > 0$ in 8.3.2., will satisfy the following limit property: If $W^{\varepsilon}_{\psi(\frac{t}{\varepsilon})} \to \Lambda_t$ in S_3' (and some regularity assumptions), then

$$\partial_t \Lambda_t + \bar{v}(2\pi \bar{k}) \cdot \nabla_{\bar{k}} \Lambda_t = 0$$

where $\bar{v}(\bar{p}) := \frac{\bar{p}}{\sqrt{\bar{p}^2 + m^2}}$. (By Theorem 8.3.7. the same result holds for H_0 using $\bar{v}(\bar{p}) = \bar{p}$, even without taking any scaling limits.)

Therefore, the physical interpretation of the Fourier variable $\bar{p} = 2\pi\bar{k}$ in this case is to identify it with the spatial part of the "momentum four-vector", as defined in special relativity. (Details are left for the "final project".)

c) Spin has non-trivial interaction with the magnetic field. The standard way to model these to electrons is to change in either $H_0 = \frac{1}{2m}\hat{p}^2$ or in $H_{rel} = \sqrt{\hat{p}^2 + m^2}$

$$\hat{p}^2 \to \left[\sum_{j=1}^{3} \hat{\sigma}_j \left(-i\partial_j + q_e A_j(x) \right) \right]^2$$

where $\hat{\sigma}_j \in \mathbb{C}^{2\times 2}$ denote the Pauli matrices defined on p. 27; they determine the action of H on the spin components of $\psi \in L^2(\mathbb{R}^3, \mathbb{C}^2)$.