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

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

$$= H_0 + \alpha V_c$$

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 $\psi \in S_{3N}$ and $F \in L^2(\mathbb{R}^3)$, $O \in O(3N)$. Then

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

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

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

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 $\psi \in S \Rightarrow g_{y'}(z) = \int_{\mathbb{R}^{3N}} dp\, e^{i 2\pi p \cdot O^T(z,y')} \hat{\psi}(p)$

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

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

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

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

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

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 $g_{y'} \in S_3$ $\forall y'$ (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.

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

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

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

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

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

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

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

This proves that if $\varepsilon > 0$, $\exists C_\varepsilon \geq 0$ s.t. $\forall \psi \in S_{3N}$, $j = 1, \dots, J$, 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 $\psi \in S_{3N}$.

Since 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 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 $\exists \psi_n \in S$ 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 $\int dx\, |\alpha V \psi|^2$ $= \int dx \left(\liminf_{n\to\infty} |\alpha V(x)\psi_n(x)|^2 \right) \leq \liminf_{n\to\infty} \int dx\, |\alpha V \psi_n|^2 \leq (a\|H_0\psi\| + b\|\psi\|)^2$ $< \infty$. This 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 $F(\bar{p}) = m + \frac{1}{2m} \bar{p}^2 + \mathcal{O}(\bar{p}^4)$

$\Rightarrow H_{rel} = m \mathbb{1} + H_0 +$ "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 $\psi \in L^2(\mathbb{R}^3, \mathbb{C}^2)$.