MATHEMATICAL TOPICS
IN MANY BODY QUANTUM THEORY

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Contents

1 Unbounded self-adjoint operators

1.1 Unbounded operators

Let $\mathcal{H}$ be a Hilbert space. We say that H is a *bounded operator* on $\mathcal{H}$ if it is a linear map $H : \mathcal{H} \to \mathcal{H}$ such that

$$\|H\| := \sup\{\|Hu\| \ : \ u \in \mathcal{H}\} < \infty. \tag{1.1}$$

We say that H is an *unbounded operator* on $\mathcal{H}$ if $H : \mathrm{Dom}(H) \to \mathcal{H}$ is a linear map, where $\mathrm{Dom}(H)$ is a linear subspace of $\mathcal{H}$ (usually dense) called the *domain of* H, and

$$\sup\{\|Hu\| \ : \ u \in \mathrm{Dom}(H)\} = \infty. \tag{1.2}$$

Note that if $\mathrm{Dom}(H) = \mathcal{H}$ and (1.2) holds, then H is pathological (not closed—this follows from Banach's Closed Graph Theorem).

Saying "an operator on $\mathcal{H}$" we will usually mean either an "unbounded operator on $\mathcal{H}$" or a "bounded operator on $\mathcal{H}$". For bounded operators, as a rule we assume that the domain is the whole $\mathcal{H}$.

1.2 Spectrum

We say that $z \in \mathbb{C}$ belongs to the *resolvent set* of H, denoted $\mathrm{rs}(H)$, if

$$(z - H) : \mathrm{Dom}(H) \to \mathcal{H} \tag{1.3}$$

is bijective and its inverse is bounded. The spectrum of H is $\mathrm{sp}(H) := \mathbb{C}\backslash\mathrm{rs}(H)$.

We say that λ belongs to the *point spectrum* of H, denoted $\mathrm{sp}_{\mathrm{p}}(H)$, if there exists $u \in \mathrm{Dom}(H)$, $u \neq 0$, such that $Hu = \lambda u$. Clearly, $\mathrm{sp}_{\mathrm{p}}(H) \subset \mathrm{sp}(H)$.

Let H_1, H_2 be two operators. We say that $H_1 \subset H_2$ (H_2 is an *extension* of H_1) if $\mathrm{Dom}(H_1) \subset \mathrm{Dom}(H_2)$ and

$$H_2\Big|_{\mathrm{Dom}(H_1)} = H_1. \tag{1.4}$$

Proposition 1.1 *If $H_1 \subsetneq H_2$, then $\mathrm{rs}(H_1) \cap \mathrm{rs}(H_2) = \emptyset$.*

Proof. If $(z - H_1) : \mathrm{Dom}(H_1) \to \mathcal{H}$ is bijective, then $(z - H_2) : \mathrm{Dom}(H_2) \to \mathcal{H}$ is not injective.

If $(z - H_2) : \mathrm{Dom}(H_2) \to \mathcal{H}$ is bijective, then $(z - H_1) : \mathrm{Dom}(H_1) \to \mathcal{H}$ is not surjective. □

1.3 Hermitian and self-adjoint operators

We say that an operator H is *Hermitian* (*symmetric*) if

$$(u|Hv) = (Hu|v), \quad u, v \in \mathrm{Dom}(H). \tag{1.5}$$

Theorem 1.2 *Let H be Hermitian. Then one of the following statements holds:*

(i) $\mathrm{sp}(H) = \mathbb{C}$.

(ii) $\mathrm{sp}(H) = \{\mathrm{Im} z \geq 0\}$.

(iii) $\mathrm{sp}(H) = \{\mathrm{Im} z \leq 0\}$.

(iv) $\mathrm{sp}(H) \subset \mathbb{R}$.

We say that H is *self-adjoint* if it is Hermitian and $\mathrm{sp}(H) \subset \mathbb{R}$.

Proposition 1.3 *If H is Hermitian H, and $z \notin \mathbb{R}$, then $(z-H) : \mathrm{Dom}(H) \to \mathcal{H}$ is injective.*

Proof. Let $z = x + \mathrm{i}y$ and $u \in \mathrm{Dom}(H)$. Then

$$\|(z - H)u\|^2 = y^2\|u\|^2 + \|(x - H)u\|^2 \geq y^2\|u\|^2. \tag{1.6}$$

Let $z \notin \mathbb{R}$, so that $y \neq 0$, and $u \neq 0$. Then $Hu \neq 0$. □

Proposition 1.4 *Let $H_1 \subsetneq H_2$ be both Hermitian. Then H_1 is not self-adjoint.*

Proof. Suppose that H_1 is self-adjoint. Then for $z \notin \mathbb{R}$, $(z - H_1) : \mathrm{Dom}(H_1) \to \mathcal{H}$ is bijective. Then $(z - H_2) : \mathrm{Dom}(H_2) \to \mathcal{H}$ is not injective. But this contradicts Prop. 1.3 □

Thus to make a self-adjoint operator from a Hermitian operator H_0 we need to extend it, and not restrict it. We have 3 options:

(i) There exists a unique self-adjoint operator H such that $H_0 \subset H$.

(ii) There exist many self-adjoint operators H such that $H_0 \subset H$.

(iii) There exists no self-adjoint operator H such that $H_0 \subset H$.

We say that H_0 is *essentially self-adjoint* if (1) holds. $\mathrm{Dom}(H_0)$ is then called a *core* (*essential domain*) of H.

Self-adjoint operators have good functional calculus. If f is any Borel function on $\mathrm{sp}(H)$, we can define $f(H)$.

Of particular importance are

- *Resolvent at $z \notin \mathrm{sp}(H)$*, $(z - H)^{-1}$.
- *Spectral projection onto a Borel set $\Xi \subset \mathrm{sp}(H)$*, $\mathbb{1}_\Xi(H)$.
- The exponential function $\mathrm{e}^{\mathrm{i}tH}$.

$$\mathbb{R} \ni t \mapsto \mathrm{e}^{\mathrm{i}tH} \in U(\mathcal{H})$$

is the unitary group generated by H. Conversely, by the Stone Theorem, every strongly continuous unitary group is of this form.

1.4 Examples of operators

We give a few examples of unbounded operators. First we give an expression defining formally the operator. Then we give a few possible domains.

Example 1.5 *Consider the Hilbert space $L^2(\mathbb{R}^d)$. Let $\mathbb{R}^d \ni k \mapsto a(k)$ be a continuous, possibly unbounded function. We set*

$$Au(k) := a(k)u(k) \tag{1.7}$$

on the following domains:

(i) $C_{\rm c}^\infty(\mathbb{R}^d)$.

(ii) $C_{\rm c}(\mathbb{R}^d)$.

(iii) $\{u \in L^2(\mathbb{R}^d) \ : \ au \in L^2(\mathbb{R}^d)\}$.

(i), (ii), (iii) are Hermitian. (i) and (ii) are essentially self-adjoint but not self-adjoint. (iii) is self-adjoint.

Example 1.6 *Consider the Hilbert space $L^2(\mathbb{R}^d)$ and the Laplacian $-\Delta$ with the following domains:*

(i) $C_{\rm c}^\infty(\mathbb{R}^d)$.

(ii) $C_{\rm c}^2(\mathbb{R}^d)$.

(iii) $\{u \in L^2(\mathbb{R}^d) \ : \ -\Delta u \in L^2(\mathbb{R}^d)\}$.

(i), (ii), (iii) are Hermitian. (i) and (ii) are essentially self-adjoint but not self-adjoint. (iii) is self-adjoint. To see this we use the Fourier transformation

$$\mathcal{F}(-\Delta u)(k) = k^2 \mathcal{F}u(k), \tag{1.8}$$

which essentially reduces this example to a special case of the previous one.

Example 1.7 *Consider now the space $L^2[0,\pi]$ and the Laplacian $-\Delta = -\partial_x^2$ with the following domains:*

(i) $C_{\rm c}^\infty(]0,\pi[)$.

(ii) $\{u \in C^\infty([0,\pi]) \ : \ u(0) = u(\pi) = 0\}$.

(iii) $\{u \in L^2[0,\pi] \ : \ u'' \in L^2[0,\pi], \ u(0) = u(\pi) = 0\}$.

(iv) $\{u \in C^\infty([0,\pi]) \ : \ u'(0) = u'(\pi) = 0\}$.

(v) $\{u \in L^2[0,\pi] \ : \ \ u'' \in L^2[0,\pi], \ u'(0) = u'(\pi) = 0\}$.

(vi) $C_{\rm c}^\infty([0,\pi])$.

(i)–(v) are Hermitian. (i) has many self-adoint extensions. (ii) is essentially self-adjoint and its self-adjoint extension is (iii). (iv) is essentially self-adjoint and its self-adjoint extension is (v). (vi) is not Hermitian.

We will denote by $-\Delta_{\rm D}$ the Laplacian $-\Delta$ with domain (iii). We will denote by $-\Delta_{\rm N}$ the Laplacian $-\Delta$ with domain (v).

Example 1.8 *Consider the space* $L^2[0,\infty[$ *and the momentum operator* $p = \frac{1}{\mathrm{i}}\partial_x$ *on the following domains:*

(i) $C_{\mathrm{c}}^{\infty}(]0,\infty[)$.

(ii) $\{u \in L^2[0,\infty[\,:\; u' \in L^2[0,\infty[,\; u(0)=0\}$.

(iii) $\{u \in L^2[0,\infty[\,:\; u'' \in L^2[0,\infty[\}$.

(i), (ii) are Hermitian but not self-adjoint. They do not possess self-adjoint extensions. (*iii*) *is not.*

We have $\mathrm{sp}(p_{(ii)}) = \{\mathrm{Im}z < 0\}$, $\mathrm{sp}_{\mathrm{p}}(p_{(ii)}) = \emptyset$,

$$R_{(ii)}(z,x,y) = \mathrm{i}\mathrm{e}^{\mathrm{i}z(x-y)}\theta(x-y), \quad \mathrm{Im}z > 0.$$

We have $\mathrm{sp}(p_{(iii)}) = \mathrm{sp}_{\mathrm{p}}(p_{(iii)}) = \{\mathrm{Im}z > 0\}$,

$$R_{(iii)}(z,x,y) = -\mathrm{i}\mathrm{e}^{\mathrm{i}z(x-y)}\theta(y-x), \quad \mathrm{Im}z < 0.$$

Lemma 1.9 *Let* $f, f' \in L^2[a,b]$. *Then* $f \in C[a,b]$ *and*

$$|f(x)| \leq C\big(\|f'\|_2 + \|f\|_2\big). \tag{1.9}$$

Proof. We use the Schwarz inequality, then we average over $[a,b]$, then again the Schwarz inequality.

$$|f(x)| = \Big|\int_z^x f'(y)\mathrm{d}y + f(z)\Big| \leq \Big(\int_z^x \mathrm{d}y\Big)^{\frac{1}{2}}\Big(\int_z^x |f'(y)|^2\mathrm{d}y\Big)^{\frac{1}{2}} + |f(z)| \tag{1.10}$$

$$\leq |b-a|^{\frac{1}{2}}\|f'\|_2 + |b-a|^{-1}\int_a^b |f(z)|\mathrm{d}z \tag{1.11}$$

$$\leq |b-a|^{\frac{1}{2}}\|f'\|_2 + |b-a|^{-\frac{1}{2}}\|f\|_2. \tag{1.12}$$

□

1.5 Operators bounded from below

We say that an operator H is positive if

$$0 \leq (u|Hu), \quad u \in \mathrm{Dom}(H). \tag{1.13}$$

If H is positive and self-adjoint, then $\mathrm{sp}(H) \subset [0,\infty[$. Therefore, we can define $H^{\frac{1}{2}}$. We can write

$$(u|Hu) = \|H^{\frac{1}{2}}u\|^2. \tag{1.14}$$

If H is unbounded, then $H^{\frac{1}{2}}$ has a bigger domain than H. We define the quadratic form associated with H as

$$h(u) := \|H^{\frac{1}{2}}u\|^2, \quad u \in \mathrm{Dom}(H^{\frac{1}{2}}). \tag{1.15}$$

We will usually abuse the notation and write $(u|Hu)$ for $h(u)$. $\mathrm{Dom}H^{\frac{1}{2}}$ is called the form domain of H and sometimes denoted $\mathcal{Q}(H)$. Thus we will write

$$h(u) = (u|Hu), \quad u \in \mathcal{Q}(H). \tag{1.16}$$

We say that H is bounded from below if there exists c such that

$$-c\|u\|^2 \leq (u|Hu), \quad u \in \mathrm{Dom}(H). \tag{1.17}$$

We can repeat essentially everything above for bounded from below operators. In particular, the form domain can be defined as $\mathrm{Dom}\big((H+c)^{\frac{1}{2}}\big)$, or what is the same $\mathrm{Dom}|H|^{\frac{1}{2}}$. For u in the form domain we can write $(u|Hu)$.

Let A, B be two operators bounded from below. We say that $A \leq B$ if $\mathrm{Dom}A \supset \mathrm{Dom}B$ and

$$(u|Au) \leq (u|Bu), \quad u \in \mathrm{Dom}B. \tag{1.18}$$

The form domain of $-\Delta_{\mathrm{D}}$ is

$$\mathcal{Q}(-\Delta_{\mathrm{D}}) = \{u \in L^2[0,\pi] \ : \ u' \in L^2[0,\pi], \quad u(0) = u(\pi) = 0\}, \tag{1.19}$$

$$(u|\Delta_{\mathrm{D}}u) = \int_0^\pi |u'(x)|^2 \mathrm{d}x, \quad u \in \mathcal{Q}(-\Delta_{\mathrm{D}}). \tag{1.20}$$

The form domain of $-\Delta_{\mathrm{N}}$ is

$$\mathcal{Q}(-\Delta_{\mathrm{N}}) = \{u \in L^2[0,\pi] \ : \ u' \in L^2[0,\pi]\}, \tag{1.21}$$

$$(u|\Delta_{\mathrm{N}}u) = \int_0^\pi |u'(x)|^2 \mathrm{d}x, \quad u \in \mathcal{Q}(-\Delta_{\mathrm{D}}). \tag{1.22}$$

Thus $\mathcal{Q}(-\Delta_{\mathrm{D}}) \subset \mathcal{Q}(-\Delta_{\mathrm{N}})$ and for $u \in \mathcal{Q}(-\Delta_{\mathrm{D}})$

$$(u|\Delta_{\mathrm{D}}u) = (u|\Delta_{\mathrm{N}}u). \tag{1.23}$$

Hence,

$$-\Delta_{\mathrm{N}} \leq -\Delta_{\mathrm{D}}. \tag{1.24}$$

1.6 Discrete and essential spectrum

Let H be selfadjoint. We partition $\mathrm{sp}(H)$ into two disjoint subsets:

$$\mathrm{sp}_{\mathrm{d}}(H) := \{\lambda \in \mathrm{sp}(H) \ : \ \exists_{\epsilon>0} \ \dim \mathbb{1}_{[\lambda-\epsilon,\lambda+\epsilon]}(H) < \infty\}, \tag{1.25}$$

$$\mathrm{sp}_{\mathrm{ess}}(H) := \{\lambda \in \mathrm{sp}(H) \ : \ \forall_{\epsilon>0} \ \dim \mathbb{1}_{[\lambda-\epsilon,\lambda+\epsilon]}(H) = \infty\}. \tag{1.26}$$

Proposition 1.10 *Let v_n be a sequence of vectors such that* $\mathrm{w}-\lim_{n\to\infty} v_n = 0$, $\|v_n\| = 1$ *and* $\lim_{n\to\infty} \|(H-\lambda)v_n\| = 0$. *Then* $\lambda \in \mathrm{sp}_{\mathrm{ess}}(H)$.

1.7 The mini-max and max-min principle

Let H be a bounded from below self-adjoint operator on a Hilbert space $\mathcal{V}$. We define

$$\begin{aligned}\mu_n(H) &:= \inf\big\{\sup\{(v|Hv)\ :\ \|v\|=1,\ v\in\mathcal{L}\}\ :\\ &\qquad \mathcal{L}\ \text{ is an } n\text{-dim. subspace of } \mathcal{V}\big\},\quad n=1,2,\dots;\\ \Sigma(H) &:= \inf \mathrm{sp}_{\mathrm{ess}}(H),\\ N(H) &:= \dim \mathbb{1}_{]-\infty,\Sigma[}(H)\end{aligned}$$

Theorem 1.11 *$\mu_n(H)$ for $n\le N$ are the consecutive eigenvalues of H, counting the multiplicity. For $n>N$ we have $\mu_n(H)=\Sigma$.*

Proof. For any $(n+1)$-dimensional space $\mathcal{L}$ there exists an n-dimensional space $\mathcal{L}'$ contained in $\mathcal{L}$. Clearly,

$$\sup\{(v|Hv)\ :\ \|v\|=1,\ v\in\mathcal{L}'\}\le\sup\{(v|Hv)\ :\ \|v\|=1,\ v\in\mathcal{L}\}.$$

Therefore, $\mu_n\le\mu_{n+1}$.

Let $a,b\in\mathrm{sp}(H)$, $]a,b[\cap\mathrm{sp}(H)=\emptyset$ and $\dim\mathbb{1}_{]-\infty,a]}(H)=n$. Let $\mathcal{L}_a:=\mathrm{Ran}\mathbb{1}_{]-\infty,a]}(H)$. Then

$$\sup\{(v|Hv)\ :\ \|v\|=1,\ v\in\mathcal{L}_a\}=a.$$

Thus $\mu_n\le a$.

If $\mathcal{L}$ is $(n+1)$-dimensional, then $\mathcal{L}\cap\mathcal{L}_a^\perp\neq\{0\}$. Thus we can find a normalized $w\in\mathcal{L}\cap\mathcal{L}_a^\perp$. Now $w\in\mathrm{Ran}\mathbb{1}_{[b,\infty[}(H)$, hence $(w|Hw)\ge b$. Thus

$$\sup\{(v|Hv)\ :\ \|v\|=1,\ v\in\mathcal{L}\}\ge b.$$

Hence, $b\le\mu_{n+1}$. □

Theorem 1.12 (The Rayleigh-Ritz method) *Let $\mathcal{W}$ be a linear subspace. Set $H_{\mathcal{W}}:=P_{\mathcal{W}}HP_{\mathcal{W}}\big|_{\mathcal{W}}$, where $P_{\mathcal{W}}$ denotes the projector onto $\mathcal{W}$. Then $H_{\mathcal{W}}$ is a bounded self-adjoint operator and*

$$\mu_n(H)\le\mu_n(H_{\mathcal{W}}).$$

Theorem 1.13 (i) *Let $H\le G$. Then $\mu_n(H)\le\mu_n(G)$.*

(ii) $|\mu_n(H)-\mu_n(G)|\le\|H-G\|$.

1.8 Weyl Theorem on essential spectrum

An operator on a Hilbert space is compact if it can be approximated in norm by finite rank operators.

All operators on finite dimension spaces are compact. In infinite dimension, a self-adjoint operator is compact iff its essential spectrum is $\{0\}$.

Theorem 1.14 *Suppose H_0, H are self-adjoint and for all $z \in \mathbb{C}\backslash\mathbb{R}$,*

$$(z-H)^{-1} - (z-H_0)^{-1}$$

is compact. Then $\mathrm{sp}_{\mathrm{ess}}(H) = \mathrm{sp}_{\mathrm{ess}}(H_0)$.

Proof. We have for $z_0 \in \mathbb{C}\backslash\mathbb{R}$ and $r < \mathrm{Im} z_0$,

$$(z_0 - H)^{-n} = \frac{1}{2\pi \mathrm{i} n!} \int_{\partial K(z_0,r)} (z_0 - z)^{-n} (z-H)^{-1} \mathrm{d}z. \tag{1.27}$$

Hence

$$(z_0-H)^{-n} - (z_0-H_0)^{-n} = \frac{1}{2\pi \mathrm{i} n!} \int_{\partial K(z_0,r)} (z_0-z)^{-n} \Big((z-H)^{-1} - (z-H_0)^{-1} \Big) \mathrm{d}z$$

is compact as well. But every $f \in C_{\mathrm{c}}(\mathbb{R})$ can be approximated in the supremum norm by linear combinations of $(z_0 - H)^{-n}$, $(\overline{z}_0 - H)^{-n}$, $n = 1, 2, \ldots$. Hence $f(H) - f(H_0)$ is compact.

In particular, let $\lambda \notin \mathrm{sp}_{\mathrm{ess}}(H)$. Then there exists $f \in C_{\mathrm{c}}(\mathbb{R})$, $f(\lambda) \neq 0$ such that $f(H)$ is compact. But $f(H) - f(H_0)$ is compact. Hence $f(H_0)$ is compact. Hence $\lambda \notin \mathrm{sp}_{\mathrm{ess}}(H_0)$. Therefore, $\mathrm{sp}_{\mathrm{ess}}(H_0) \subset \mathrm{sp}_{\mathrm{ess}}(H)$. □

2 Schrödinger operators

2.1 Stability of essential spectrum

Theorem 2.1 *Suppose now that V is a bounded real function and*

$$H_0 = -\Delta, \ H = -\Delta + V(x).$$

Obviously, H is self-adjoint on $\mathrm{Dom}(H_0)$ *and bounded from below.*

Assume in addition that $\lim_{|x|\to\infty} V(x) = 0$. *Then*

$$\mathrm{sp}_{\mathrm{ess}}(H) = [0, \infty[.$$

Proof.

$$(z-H)^{-1} - (z-H_0)^{-1} = (z-H)^{-1} V(x) (z-H_0)^{-1}$$

is compact, because $V(x)(z-H_0)^{-1}$ is compact. Besides, $\mathrm{sp}_{\mathrm{ess}}(H_0) = \mathrm{sp}(H_0) = [0, \infty[$. □

2.2 Confining potentials

Theorem 2.2 *Let* $\lim_{|x|\to\infty} V(x) = \infty$ *and* $H = -\Delta + V(x)$. *Then* $\mathrm{sp}_{\mathrm{ess}}(H) = \emptyset$.

Proof. Let $\lambda \in \mathbb{R}$. Set $V_\lambda := \min(V, \lambda)$. We have

$$H \geq H_\lambda := -\Delta + V_\lambda$$

and by Thm 2.1, $\mathrm{sp}_{\mathrm{ess}} H_\lambda = [\lambda, \infty[$. Therefore, $\mathrm{sp}_{\mathrm{ess}} H \subset [\lambda, \infty[$. □

Here is an alternative proof:

Proof. We can assume that $V(x) \geq 0$.

$$1 + H \geq 1 - \Delta, \tag{2.28}$$
$$1 + H \geq 1 + V(x). \tag{2.29}$$

Hence

$$\mathbb{1} \geq (1+H)^{-\frac{1}{2}}(1-\Delta)(1+H)^{-\frac{1}{2}}, \tag{2.30}$$
$$\mathbb{1} \geq (1+H)^{-\frac{1}{2}}(1+V(x))(1+H)^{-\frac{1}{2}}. \tag{2.31}$$

Therefore,

$$1 \geq \left\|(1-\Delta)^{\frac{1}{2}}(1+H)^{-\frac{1}{2}}\right\|, \tag{2.32}$$
$$1 \geq \left\|(1+V(x))^{\frac{1}{2}}(1+H)^{-\frac{1}{2}}\right\|. \tag{2.33}$$

Now

$$(1+H)^{-1} \tag{2.34}$$
$$= (1+H)^{-\frac{1}{2}}(1+V(x))^{\frac{1}{2}}(1+V(x))^{-\frac{1}{2}}(1-\Delta)^{-\frac{1}{2}}(1-\Delta)^{\frac{1}{2}}(1+H)^{-\frac{1}{2}}$$

and $(1+V(x))^{-\frac{1}{2}}(1-\Delta)^{-\frac{1}{2}}$ is compact. Hence $(1+H)^{-1}$ is compact. □

2.3 Weyl asymptotics

For a bounded from below self-adjoint operator H set

$$N_\mu(H) := \#\{\text{eigenvalues of } H \text{ counted with multiplicity } \leq \mu\} \tag{2.35}$$
$$= \mathrm{Tr}\mathbb{1}_{]-\infty,\mu]}(H). \tag{2.36}$$

We will show that if V is continuous potential with $V - \mu > 0$ outside a compact set then

$$N_\mu(-\hbar^2\Delta + V(x)) \simeq (2\pi\hbar)^{-d} c_d \int_{V(x)\leq\mu} |V(x) - \mu|_-^{\frac{d}{2}} \mathrm{d}x + o(\hbar^{-d}) \tag{2.37}$$
$$= (2\pi\hbar)^{-d} \int_{h(x,p)\leq\mu} \mathrm{d}x\mathrm{d}p + o(\hbar^{-d}). \tag{2.38}$$

Asymptotics of this form is called the *Weyl asymptotics*.

Here are the tools that we will use:

$$A \leq B \;\Rightarrow\; N_\mu(A) \geq N_\mu(B),$$

$$N_\mu(A \oplus B) = N_\mu(A) + N_\mu(B).$$

To simplify we will assume that $d = 1$.

Lemma 2.3 *Let $\Delta_{[0,L],D}$, resp. $\Delta_{[0,L],N}$ denote the Dirichlet, resp. Neumann Laplacian on $[0, L]$. For $\alpha \in \mathbb{R}$ let $[\alpha]$ denote the largest integer $\leq \alpha$, $\theta(\alpha)$ the Heavyside function and $|\mu|_+ := \mu\theta(\mu)$. Then*

$$\begin{aligned} N_\mu\big(-\hbar^2\Delta_{[0,L],D}\big) &= [L(\pi\hbar)^{-1}|\mu|_+^{1/2}], \\ N_\mu\big(-\hbar^2\Delta_{[0,L],N}\big) &= [L(\pi\hbar)^{-1}|\mu|_+^{1/2}] + \theta(\mu). \end{aligned}$$

Proof. The eigenfunctions and the spectrum of $\Delta_{[0,L],D}$, resp. $\Delta_{[0,L],N}$ are

$$\begin{aligned} &\sin\frac{\pi n x}{L}, \qquad \frac{\hbar^2\pi^2 n^2}{L^2}, \quad n = 1, 2, \dots; \\ &\cos\frac{\pi n x}{L}, \qquad \frac{\hbar^2\pi^2 n^2}{L^2}, \quad n = 0, 1, 2, \dots. \end{aligned}$$

Thus the last eigenvalue has the number $n = [L(\hbar\pi)^{-1}|\mu|_+^{1/2}]$. □

Divide $\mathbb{R}$ into intervals

$$I_{m,j} := \Big[(j - 1/2)m^{-1}, (j + 1/2)m^{-1}\Big].$$

Put at the borders of the intervals the Neumann/Dirichlet boundary conditions. The Neumann conditions lower the expectation value and the Dirichlet conditions increase them. Set

$$\begin{aligned} \overline{V}_{m,j} &= \sup\{V(x) \;:\; x \in I_{m,j}\}, \\ \underline{V}_{m,j} &= \inf\{V(x) \;:\; x \in I_{m,j}\}. \end{aligned}$$

We have

$$\begin{aligned} & & \bigoplus_{j\in\mathbb{Z}} \Big(-\hbar^2\Delta_{I_{m,j},N} + \underline{V}_{m,j}\Big) \\ \leq\; -\hbar^2\Delta + V(x) \;\leq\; & & \bigoplus_{j\in\mathbb{Z}} \Big(-\hbar^2\Delta_{I_{m,j},D} + \overline{V}_{m,j}\Big). \end{aligned}$$

Hence,

$$\begin{aligned} & & \sum_{j\in\mathbb{Z}} N_\mu\Big(-\hbar^2\Delta_{I_{m,j},N} + \underline{V}_{m,j}\Big) \\ \geq\; N_\mu\Big(-\hbar^2\Delta + V(x)\Big) \;\geq\; & & \sum_{j\in\mathbb{Z}} N_\mu\Big(-\hbar^2\Delta_{I_{m,j},D} + \overline{V}_{m,j}\Big). \end{aligned}$$

Therefore,

$$\begin{aligned} & \sum_{j\in\mathbb{Z}} m^{-1}(\hbar\pi)^{-1}|\underline{V}_{m,j}-\mu|_-^{1/2} + \sum_{j\in\mathbb{Z}} \theta\big(\mu-\underline{V}_{m,j}\big) \\ \geq\ N_\mu\Big(-\hbar^2\Delta+V(x)\Big) \quad &\geq \quad \sum_{j\in\mathbb{Z}} m^{-1}(\hbar\pi)^{-1}|\overline{V}_{m,j}-\mu|_-^{1/2}. \end{aligned}$$

Using the fact that $|V-\mu|_-$ has a compact support, we can estimate

$$\sum_{j\in\mathbb{Z}} \theta\big(\mu-\underline{V}_{m,j}\big) \quad \leq \quad mC.$$

By properties of Riemann sums we can find m_ϵ such that for $m \geq m_\epsilon$

$$\Big|\sum_{j\in\mathbb{Z}} m^{-1}|\underline{V}_{m,j}-\mu|_-^{1/2} - \int |V(x)-\mu|_-^{1/2}\mathrm{d}x\Big| \quad < \quad \epsilon/3, \tag{2.39}$$

$$\Big|\sum_{j\in\mathbb{Z}} m^{-1}|\overline{V}_{m,j}-\mu|_-^{1/2} - \int |V(x)-\mu|_-^{1/2}\mathrm{d}x\Big| \quad < \quad \epsilon/3. \tag{2.40}$$

Therefore,

$$\Big|N_\mu\Big(-\hbar^2\Delta+V(x)\Big) - \frac{1}{\hbar\pi}\int |V(x)-\mu|_-^{1/2}\mathrm{d}x\Big| \quad < \quad \frac{2\epsilon}{\hbar\pi 3} + \frac{Cm_\epsilon}{\pi}. \tag{2.41}$$

Hence the right hand side of (2.41) is $o(\hbar^{-1})$. This proves (2.37)

If we assume that V is differentiable, then m_ϵ can be assumed to be $C_0\epsilon^{-1}$. Then we can optimize and set $\epsilon = \sqrt{\hbar}$. This allows us to replace $o(\hbar^{-1})$ by $O(\hbar^{-1/2})$.

3 Many body Schrödinger operators

3.1 Two particle Schrödinger operators

Let $X_i = \mathbb{R}^d$ be the configuration space of the ith particle. Consider the Hilbert space $\mathcal{H} := L^2(X_1 \oplus X_2)$ and the Hamiltonian

$$H = \frac{1}{2m_1}p_1^2 + \frac{1}{2m_2}p_2^2 + V(x_1-x_2).$$

Introduce

$$x_{12} := \frac{m_1x_1+m_2x_2}{m_1+m_2}, \qquad m_{12} := m_1+m_2, \tag{3.42}$$

$$x^{12} := x_1-x_2, \qquad m^{12} := \frac{1}{\frac{1}{m_1}+\frac{1}{m_2}}. \tag{3.43}$$

Then $\mathcal{H} = L^2(X_{12} \oplus X^{12}) = L^2(X_{12}) \otimes L^2(X^{12})$,

$$H = \frac{1}{m_{12}} p_{12}^2 + \frac{1}{m^{12}} (p^{12})^2 + V(x^{12}) \tag{3.44}$$

$$= \frac{1}{m_{12}} p_{12}^2 + H^{12}. \tag{3.45}$$

This can be interpreted as follows: in $X_1 \oplus X_2$ we introduce the scalar product, such that

$$\langle x_1, x_2 | x_1, x_2 \rangle = m_1 x_1^2 + m_2 x_2^2.$$

The corresponding Laplacian is

$$\frac{1}{m_1} p_1^2 + \frac{1}{m_2} p_2^2,$$

which is twice the kinetic energy.

In $X_1 \oplus X_2$ we have the collision plane

$$X_{12} := \{(x_1, x_2) \in X_1 \oplus X_2 \ : \ x_1 = x_2\}.$$

Define X^{12} to be the orthogonal complement of X_{12} wrt this product. X_{12} is spanned by (x, x) and X^{12} by $(m_2 x, -m_1 x)$. We check that

$$\{x_{12} = 0\} = X^{12}, \tag{3.46}$$

$$\{x^{12} = 0\} = X_{12}. \tag{3.47}$$

Moreover,

$$\begin{aligned} & m_{12} x_{12}^2 + m^{12} (x^{12})^2 \\ =& \frac{1}{m_1 + m_2} (m_1^2 x_1^2 + 2 m_1 m_2 x_1 x_2 + m_2^2 x_2^2) + \frac{m_1 m_2}{m_1 + m_2} (x_1^2 - 2 x_1 x_2 + x_2^2) \\ =& m_1 x_1^2 + m_2 x_2^2. \end{aligned}$$

Therefore,

$$\frac{1}{m_{12}} p_{12}^2 + \frac{1}{m^{12}} (p^{12})^2 = \frac{1}{m_1} p_1^2 + \frac{1}{m_2} p_2^2.$$

3.2 3-body Schrödinger Hamiltonian

Consider $\mathcal{H} := L^2(X_1 \oplus X_2 \oplus X_3)$ and the Hamiltonian

$$H = \sum_{i=1}^{3} \frac{1}{2m_i} p_i^2 + \sum_{1 \le i < j \le 3} V_{ij}(x_i - x_j).$$

Introduce the Jacobi coordinates:

$$x^{12} := x_1 - x_2, \qquad m^{12} := \frac{1}{\frac{1}{m_1} + \frac{1}{m_2}},$$

$$x^3 := \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2} - x_3, \qquad m^3 := \frac{1}{\frac{1}{m_1+m_2} + \frac{1}{m_3}},$$

$$x_{123} := \frac{m_1 x_1 + m_2 x_2 + m_3 x_3}{m_1 + m_2 + m_3}, \qquad m_{123} := m_1 + m_2 + m_3.$$

We have

$$x^2 := m_1 x_1^2 + m_2 x_2^2 + m_3 x_3^2 = m_{123} x_{123}^2 + m^3 (x^3)^2 + m^{12} (x^{12})^2, \tag{3.48}$$

$$p^2 := \frac{1}{m_1} p_1^2 + \frac{1}{m_2} p_2^2 + \frac{1}{m_3} p_3^2 = \frac{1}{m_{123}} p_{123}^2 + \frac{1}{m^3} (p^3)^2 + \frac{1}{m^{12}} (p^{12})^2. \tag{3.49}$$

We have the 3-body collision plane

$$X_{123} := \{(x_1, x_2, x_3) \ : \ x_1 = x_2 = x_3\}.$$

and 3 2-body collision planes

$$X_{ij} := \{(x_1, x_2, x_3) \ : \ x_i = x_j\}.$$

Let us write $X^{123} := X_{123}^{\perp}$, $X^{ij} := X_{ij}^{\perp}$. Clearly, $X_{123} \subset X_{ij}$, hence $X_{123} \perp X^{ij}$.

Set $X^3 := X^{123} \cap X_{12}$. Clearly, $X = X_{123} \oplus X^3 \oplus X^{12}$. We claim that this notation is consistent with previous coordinates. Indeed,

$$\begin{aligned}
X_{123} &= \{(x_1, x_2, x_3) \mid x^3 = x^{12} = 0\} \\
&\quad \text{is spanned by } z_{123} := \frac{1}{m_{123}}(1,1,1), \quad \|z_{123}\|^2 = \frac{1}{m_{123}}, \\
X^3 &= \{(x_1, x_2, x_3) \mid x_{123} = x^{12} = 0\} \\
&\quad \text{is spanned by } z^3 := \Big(\frac{1}{m_1 + m_2}, \frac{1}{m_1 + m_2}, -\frac{1}{m_3}\Big), \quad \|z^3\|^2 = \frac{1}{m^3}, \\
X^{12} &= \{(x_1, x_2, x_3) \mid x_{123} = x^3 = 0\} \\
&\quad \text{is spanned by } z^{12} := \Big(\frac{1}{m_1}, -\frac{1}{m_2}, 0\Big), \quad \|z^{12}\|^2 = \frac{1}{m^{12}}.
\end{aligned}$$

Now (3.48) is simply

$$x^2 = \frac{(z^{12}|x)^2}{\|z^{12}\|^2} + \frac{(z^3|x)^2}{\|z^3\|^2} + \frac{(z_{123}|x)^2}{\|z_{123}\|^2}. \tag{3.50}$$

We can separate the center of mass motion:

$$\mathcal{H} = L^2(X_{123}) \otimes L^2(X^3 \oplus X^{12}) \tag{3.51}$$

$$H = \frac{1}{2m_{123}} p_{123}^2 + \frac{1}{2m^3} (p^3)^2 + \frac{1}{2m^{12}} (p^{12})^2 + \sum_{1 \le i < j \le 3} V_{ij}(x_i - x_j) \tag{3.52}$$

$$= \frac{1}{2m_{123}} p_{123}^2 + H^{123}. \tag{3.53}$$

We can also introduce the Hamiltonian of the pair (ij) and separate its center of mass motion:

$$\mathcal{H} = L^2(X_{123} \oplus X^3) \otimes L^2(X^{12}) \tag{3.54}$$

$$H_{12} = \sum_{i=1}^{3} \frac{1}{2m_i} p_i^2 + V_{12}(x_1 - x_2), \tag{3.55}$$

$$= \frac{1}{2m_{123}} p_{123}^2 + \frac{1}{2m^3}(p^3)^2 + H^{12}. \tag{3.56}$$

3.3 N-body Schrödinger Hamiltonians

Consider $\mathcal{H} := L^2(X_1 \oplus \cdots \oplus X_n) = L^2(X)$ and the Hamiltonian

$$H = \sum_{i=1}^{n} \frac{1}{2m_i} p_i^2 + \sum_{1 \le i < j \le n} V_{ij}(x_i - x_j). \tag{3.57}$$

The configuration space $X_1 \oplus \cdots \oplus X_n$ is equipped with the scalar product

$$\langle x_1, \ldots, x_n | x_1, \ldots, x_n \rangle = \sum_{i=1}^{n} m_i x_i^2.$$

The kinetic energy is half the Laplacian wrt this product:

$$-\Delta := \sum_{i=1}^{n} \frac{1}{m_i} p_i^2.$$

We will say cluster for a subset of $\{1, \ldots, n\}$. An example of a cluster is a pair (ij). We define the collision plane corresponding to a cluster c:

$$X_c := \{(x_1, \ldots, x_n) \ : \ x_i = x_j, \ i, j \in c\}.$$

We set $X^c := X_c^{\perp}$. For every cluster $c \subset \{1, \ldots, n\}$ we have the factorization of the Hilbert space into internal and external degrees of freedom and we define the full cluster Hamiltonian H_c and the internal cluster Hamiltonian H^c:

$$\mathcal{H} = L^2(X_c) \otimes L^2(X^c), \tag{3.58}$$

$$H_c := -\frac{1}{2}\Delta + \sum_{i,j \in c} V_{ij}(x_i - x_j) \tag{3.59}$$

$$= -\frac{1}{2}\Delta_c - \frac{1}{2}\Delta^c + V_c(x^c) \ = \ -\frac{1}{2}\Delta_c + H^c. \tag{3.60}$$

For instance

$$H = H_{\{1,\ldots,n\}} = -\frac{1}{2}\Delta_{\{1,\ldots,n\}} + H^{\{1,\ldots,n\}}$$

is the separation of the full center-of-mass motion.

A cluster decomposition is a partition of $\{1,\dots,n\}$ into clusters. Let a, b be cluster decompositions. We say that $b \subset a$ if b is finer than a. In particular, $\{1\},\dots\{n\}$ is minimal and $\{1,\dots,n\}$ is maximal.

For any cluster decomposition $a = \{c_1,\dots,c_k\}$ we define the corresponding collision plane

$$X_a := \bigcap_{i=1}^{k} X_{c_i} := \{(x_1,\dots,x_n) \ : \ x_i = x_j, \ (i,j) \subset a\}.$$

We set $X^a := X_a^{\perp}$.

We have the corresponding full Hamiltonian H_a and internal Hamiltonian H^a:

$$\mathcal{H} = L^2(X_a) \otimes L^2(X^a), \tag{3.61}$$

$$H_a := -\frac{1}{2}\Delta + \sum_{(i,j)\subset a} V_{ij}(x_i - x_j) \tag{3.62}$$

$$= -\frac{1}{2}\Delta_a - \frac{1}{2}\Delta^a + V_a(x^a) \ = \ -\frac{1}{2}\Delta_a + H^a. \tag{3.63}$$

Clearly,

$$X^c \subset \{(x_1,\dots,x_n) \mid x_i = 0, \quad i \notin c\}.$$

Therefore, if $c_1 \cap c_2 = \emptyset$, then $X^{c_1} \perp X^{c_2}$. Therefore, if $a = \{c_1,\dots,c_k\}$, then

$$X^a = X^{c_1} \oplus \cdots \oplus X^{c_k}. \tag{3.64}$$

$$L^2(X^a) = L^2(X^{c_1}) \otimes \cdots \otimes L^2(X^{c_k}).$$

We have

$$H^a = \sum_{i=1}^{k} H^{c_i}.$$

Note that H^a may have point spectrum.

Let $b \subset a$. Clearly, $X_b \supset X_a$, $X^b \subset X^a$. We can introduce $X_b^a := X_b \cap X^a$, so that

$$X_b = X_a \oplus X_b^a, \quad X^a = X_b^a \oplus X^b.$$

We have the corresponding Laplacian Δ_b^a, so that

$$\Delta_b = \Delta_a \oplus \Delta_b^a, \quad \Delta^a = \Delta_b^a \oplus \Delta^b.$$

We can also decompose the internal Hamiltonian:

$$L^2(X^a) = L^2(X_b^a) \otimes L^2(X^b), \tag{3.65}$$

$$H_b^a = -\frac{1}{2}\Delta^a + V_b(x^b) = -\frac{1}{2}\Delta_b^a + H^b. \tag{3.66}$$

It is also useful to introduce the "interaction"

$$I_b^a = V_a - V_b = \sum_{(i,j)\subset a,\ (ij)\not\subset b} V_{ij}(x_i - x_j),$$

so that

$$H_a = H_b + I_b^a, \tag{3.67}$$

$$H^a = -\frac{1}{2}\Delta_b^a + H^b + I_b^a. \tag{3.68}$$

3.4 The HVZ Theorem

Theorem 3.1 *Let* $E_a := \inf \mathrm{sp} H^a$. *Then*

$$\mathrm{sp}_{\mathrm{ess}} H^{\{1,\dots,n\}} = \Big[\inf_{a\neq\{1,\dots,n\}} E_a, \infty \Big[.$$

More generally

$$\mathrm{sp}_{\mathrm{ess}} H^a = \Big[\inf_{b\subsetneq a} E_b, \infty \Big[. \tag{3.69}$$

Proof. We will use the notation of (3.69), thinking of $a = \{1,\dots,n\}$.

$\supset$. Let $b \subsetneq a$ and $\lambda \in [E_b, \infty[$. Clearly, $\mathrm{sp}(-\frac{1}{2}\Delta_b^a + H^b) = [E_b, \infty[$. Hence, there exist approximate eigenfunctions of $-\frac{1}{2}\Delta_b^a + H^b$ for the eigenvalue λ. $-\frac{1}{2}\Delta_b^a + H^b$ is invariant in the direction of X_b^a. Therefore, these eigenfunctions can be moved far away from the X_{ij} with $(ij) \not\subset b$. But there I_b^a is small. By (3.68), they are approximate eigenfunctions of H^a.

$\subset$. First we claim that we can find a partition of unity $\{\chi_b \in C^\infty(X^a) \ : \ b \subsetneq a\}$ such that χ_b outside a ball are homogeneous and are zero on X_{ij} with $(ij) \not\subset b$.

There are many such partitions of unity. Indeed, consider a unit sphere S^a in X^a. For any $(x_1,\dots,x_n) \in S^a$, there exists a pair (i,j) such that $x_i \neq x_j$. If b is a 2-cluster decomposition b such that i and j belong to different clusters, then $(x_1,\dots,x_n) \notin X_b$. Therefore,

$$\{S^a \backslash X_b \mid b \text{ is a 2-cluster decomposition } \}$$

is a covering of S^a with open sets. We can choose a smooth partition of unity subordinated to this covering, then extend it by homogeneity in the outside of the ball, and by smoothness in the inside. Note that 2-cluster decompositions b satisfy $b \subsetneq a = \{1,\dots,n\}$

Now

$$\begin{aligned}(z - H^a)^{-1} &= \sum_{b\subsetneq a} (z - H^a)^{-1}\chi_b \\ &= \sum_{b\subsetneq a} (z - H_b^a)^{-1}\chi_b + \sum_{b\subsetneq a} \Big((z - H^a)^{-1} - (z - H_b^a)^{-1} \Big)\chi_b.\end{aligned}$$

Moreover,

$$\begin{aligned}\Big((z-H^a)^{-1}-(z-H_b^a)^{-1}\Big)\chi_b =&(z-H^a)^{-1}I_b^a(z-H_b^a)^{-1}\chi_b\\ =&(z-H^a)^{-1}I_b^a\chi_b(z-H_b^a)^{-1}\\ &+(z-H^a)^{-1}I_b^a[(z-H_b^a)^{-1},\chi_b]\\ =&(z-H^a)^{-1}I_b^a\chi_b(z-H_b^a)^{-1}\\ &+(z-H^a)^{-1}I_b^a(z-H_b^a)^{-1}\frac{1}{\mathrm{i}2}(p^a\nabla\chi_b+\nabla\chi_b p^a)(z-H_b^a)^{-1}.\end{aligned}$$

But $I_b^a\chi_b$ and $\nabla\chi_b$ decay at infinity and $p^a(z-H_b^a)^{-1}$ is bounded. Hence both terms on the rhs are compact.

Hence,

$$(z-H^a)^{-1}=\sum_{b\subsetneq a}(z-H_b^a)^{-1}\chi_b+\text{ compact.}$$

Repeating the argument from the proof of Thm 1.14, for $f\in C_{\mathrm{c}}(\mathbb{R})$ we obtain

$$f(H^a)=\sum_{b\subsetneq a}f(H_b^a)\chi_b+\text{ compact.}\tag{3.70}$$

Now let $\operatorname{supp} f\cap\Big[\inf_{b\subsetneq a}E_b,\infty\Big[=\emptyset$. Then $f(H_b^a)=0$. Hence $f(H^a)$ is compact. Therefore, $\operatorname{sp}_{\mathrm{ess}}(H^a)\subset\Big[\inf_{b\subsetneq a}E_b,\infty\Big[$. □

4 Scattering theory

4.1 Abstract scattering theory

Assume that H_0 and H are self-adjoint operators on a Hilbert space $\mathcal{H}$.

The *Møller* or *wave operators* (if they exist) are defined as

$$\Omega^{\pm}\;:=\;\mathrm{s}-\lim_{t\to\pm\infty}\mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}.$$

The *scattering operator* is defined as

$$S:=\Omega^{+*}\Omega^{-}.\tag{4.71}$$

Theorem 4.1 (i) *If the Møller operators exist, they are* isometric *and intertwine the free and the full Hamiltonian:* $\Omega^{\pm}H_0=H\Omega^{\pm}$.

(ii) *The scattering operator exists and commutes with the free Hamiltonian:* $H_0S=SH_0$.

Proof. $\Omega^{\pm}$ are isometric as strong limits of unitary operators.
We have

$$\mathrm{e}^{\mathrm{i}sH}\Big(\mathrm{s}-\lim_{t\to\infty}\mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}\Big)\mathrm{e}^{-\mathrm{i}sH_0} = \mathrm{s}-\lim_{t\to\pm\infty}\mathrm{e}^{\mathrm{i}(t+s)H}\mathrm{e}^{-\mathrm{i}(t+s)H_0} \tag{4.72}$$

$$= \mathrm{s}-\lim_{t\to\pm\infty}\mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}. \tag{4.73}$$

Hence,

$$\mathrm{e}^{\mathrm{i}sH}\Omega^{\pm} = \Omega^{\pm}\mathrm{e}^{\mathrm{i}sH_0}.$$

□

Theorem 4.2 *If the Møller operator exists and $H_0\Psi = E\Psi$, then $H\Psi = E\Psi$.*

Proof. Let $H_0\Psi = E\Psi$. If $\lim_{t\to\infty}\mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}\Psi$ exists, then it coincides with the limit of its exponential average:

$$\lim_{t\to\infty}\mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}\Psi = \lim_{\epsilon\searrow 0}\epsilon\int_0^{\infty}\mathrm{e}^{-\epsilon t}\mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}\Psi\mathrm{d}t$$

$$= \lim_{\epsilon\searrow 0}\epsilon\int_0^{\infty}\mathrm{e}^{t(-\epsilon+\mathrm{i}H-\mathrm{i}E)}\Psi\mathrm{d}t = \lim_{\epsilon\searrow 0}\frac{\epsilon}{(\epsilon+\mathrm{i}(E-H))}\Psi = \mathbb{1}_{\{E\}}(H)\Psi.$$

This is the reason why in practice the standard formalism of scattering theory is usually applied in situations where the unperturbed Hamiltonian H_0 has only continuous spectrum, which we will assume below.

Note that $\mathrm{Ran}\Omega^{\pm}$ is an invariant subspace of H. H can have eigenvectors, but they are orthogonal to $\mathrm{Ran}\Omega^{\pm}$. The property

$$\mathrm{Ran}\mathbb{1}_{\mathrm{p}}(H)\oplus\mathrm{Ran}\Omega^{\pm} = \mathcal{H}$$

or

$$\mathrm{Ran}\Omega^{\pm} = \mathrm{Ran}\mathbb{1}_{\mathrm{c}}(H)$$

is called asymptotic completeness. It guarantees that S is unitary.

4.2 1-body Schrödinger operators

Consider a single quantum particle in an external potential, described by the Hilbert space $L^2(\mathbb{R}^d)$ and the Schrödinger Hamiltonian.

$$H = H_0 + V(x),$$

where

$$H_0 = p^2, \quad p = \frac{1}{\mathrm{i}}\partial_x.$$

Theorem 4.3 *Assume that $V(x)$ is* short range*, that is,*

$$|V(x)| \le c\langle x\rangle^{-\mu}, \quad \mu > 1.$$

Then there exist Møller operators

$$\Omega^{\pm} := \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0},$$

They are of course isometric, intertwine H_0 and H. Besides, they are complete*:*

$$\mathrm{Ran}\Omega^{\pm} = \mathrm{Ran}\mathbb{1}_{\mathrm{c}}(H).$$

Sketch of proof of the existence. First we study the free dynamics. We show that for Φ from a dense subset in $L^2(\mathbb{R}^d)$, their free evolution $\mathrm{e}^{-\mathrm{i}tH_0}\Phi$ is for large t concentrated in $|x| \geq ct$, where $c > 0$. We will prove that

$$\lim_{t\to\infty} \mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}\Phi, \tag{4.74}$$

exists for such Φ. We compute

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}\Phi = \mathrm{i}\mathrm{e}^{\mathrm{i}tH}V(x)\mathrm{e}^{-\mathrm{i}tH_0}\Phi.$$

But for $|x| > ct$ we have $|V(x)| \leq C(1+t)^{-\mu}$, which is integrable. Therefore,

$$\int_0^{\infty} \Big\| \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}\Phi\Big\|\mathrm{d}t < \infty.$$

But

$$\Big\|\mathrm{e}^{\mathrm{i}t_2H}\mathrm{e}^{-\mathrm{i}t_2H_0}\Phi - \mathrm{e}^{\mathrm{i}t_1H}\mathrm{e}^{-\mathrm{i}t_1H_0}\Phi\Big\| \leq \int_{t_1}^{t_2} \Big\| \frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}\Phi\Big\|\mathrm{d}t.$$

Therefore,

$$t \mapsto \mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}tH_0}\Phi$$

is Cauchy. Hence, the limit (4.74) exists. □

Note that the existence part of the above theorem is quite easy. The asymptotic completeness is much more difficult.

Theorem 4.4 *Assume that $V(x)$ is* long range*, that is,*

$$V(x) = V_{\mathrm{l}}(x) + V_{\mathrm{s}}(x),$$

where $V_{\mathrm{s}}(x)$ is short range and

$$|\partial_x^{\alpha} V_{\mathrm{l}}(x)| \leq c_{\alpha}\langle x\rangle^{-|\alpha|-\mu_{\mathrm{l}}}, \quad \mu_{\mathrm{l}} > 0,\ \alpha \in \mathbb{N}^d.$$

Then there exists a function $(t,\xi) \mapsto S_t(\xi)$ and modified Møller operators

$$\Omega^{\pm} := \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH}\mathrm{e}^{-\mathrm{i}S_t(p)},$$

$\Omega^{\pm}$ are isometric, they satisfy $H\Omega^{\pm} = \Omega^{\pm}H_0$ and they are complete*:*

$$\mathrm{Ran}\Omega^{\pm} = \mathrm{Ran}\mathbb{1}_{\mathrm{c}}(H).$$

The integral kernel of S defines *scattering amplitudes*. Setting $k = |k|\hat{k}$, it can be written as

$$S(k_2,k_1) = \delta(k_1-k_2) + \delta(k_1^2-k_2^2)t(k_1^2;\hat{k}_2,\hat{k}_1), \tag{4.75}$$

where $|t(k_1^2;\hat{k}_2,\hat{k}_1)|^2$ describes the *scattering cross-section* for the process at energy $k_1^2 = k_2^2$ from the angle $\hat{k}_1$ to the angle $\hat{k}_2$.

4.3 Scattering theory for N-body Schrödinger Hamiltonians

Consider an N-body Schrödinger Hamiltonian (3.57). Introduce various objects defined in Subsection 3.3. In addition, define

$$\mathcal{H}^a := \mathrm{Ran}\mathbb{1}_{\mathrm{p}}(H^a) \simeq \mathrm{Ran}\mathbb{1}_{\mathrm{p}}(H^{c_1}) \otimes \cdots \otimes \mathrm{Ran}\mathbb{1}_{\mathrm{p}}(H^{c_k}).$$

Let

$$E^a := H^a\Big|_{\mathcal{H}^a} = H^{c_1}\Big|_{\mathcal{H}^{c_1}} + \cdots + H^{c_k}\Big|_{\mathcal{H}^{c_k}}$$

be the operator describing the *bound state energies of clusters*. Let

$$J^a : L^2(X_a) \otimes \mathcal{H}^a \to L^2(X)$$

be the embedding of *bound states of clusters* into the full Hilbert space.

Theorem 4.5 *Assume that the potentials V_{ij} are short range. Then for any cluster decompostion a there exists the corresponding* partial wave operator

$$\Omega_a^{\pm} := \mathrm{s}\text{-}\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH} J_a \mathrm{e}^{-\mathrm{i}t(-\frac{1}{2}\Delta_a + E^a)}.$$

$\Omega_a^{\pm}$ are isometric, they intertwine the cluster and the full Hamiltonian:

$$\Omega_a^{\pm}(-\frac{1}{2}\Delta_a + E^a) = H\Omega_a^{\pm}$$

and are complete:

$$\bigoplus_a \mathrm{Ran}\Omega_a^{\pm} = L^2(X).$$

Theorem 4.6 *Assume that the potentials V_{ij} are long range with*

$$\mu_{\mathrm{l}} > \sqrt{3} - 1.$$

Then for any cluster decompostion a there exists a function $(t, \xi_a) \mapsto S_{a,t}(\xi_a)$, the corresponding partial modified wave operator

$$\Omega_a^{\pm} := \mathrm{s}\text{-}\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}tH} J_a \mathrm{e}^{-\mathrm{i}(S_{a,t}(p_a) + tE^a)},$$

which satisfy the same properties as those stated in the short range case.

Note that $\Omega^{\pm}_{\{1,\dots,n\}} = \mathbb{1}_{\mathrm{p}}(H^{\{1,\dots,n\}})$.

AC means that all states in $L^2(X)$ can be decomposed into states with a clear physical/chemical interpretation such as *atoms, ions and molecules*. The partial wave operators $\Omega_a^{\pm}$ can be organized into

$$\bigoplus_a L^2(X_a) \otimes \mathcal{H}^a \ni (\psi_a) \mapsto \sum_a \Omega_a^{\pm}\psi_a \in L^2(X),$$

which is unitary.

We can introduce *partial scattering operators*

$$S_{ab} := \Omega_a^{+*}\Omega_b^-$$

describing various processes, such as *elastic and inelastic scattering, ionization, capture of an electron, chemical reactions*. The partial scattering operators S_{ab} arranged in the matrix $[S_{ab}]$ form a unitary operator on $\bigoplus_a L^2(X_a) \otimes \mathcal{H}^a$.

2-body scattering theory, including AC in both short- and long-range case, was understood already in the 60's.

Existence of N-body wave operators and the orthogonality of their ranges was established about the same time. What was missing for a long time was *Asymptotic Completeness* – the fact that the ranges of wave operators span the whole Hilbert space.

5 Scattering amplitudes and cross-sections

We will describe general rules how to compute *transition probabilities* and *scattering cross-sections* from *scattering amplitudes*, that is, matrix elements of the *scattering operator*. These rules are essentially independent of details of a quantum system and can be derived from basic quantum mechanics.

5.1 Scattering amplitude and transition probability

Suppose that S is a unitary operator on a Hilbert space $\mathcal{H}$ having the interpretation of a *scattering operator*. Suppose that the *initial state* is given by a normalized vector Φ^- and the *final measurement* by a positive operator Q^+. Then the *transition probability* is given by

$$\left(\Phi^-|S^*Q^+S\Phi^-\right) = \mathrm{Tr}\Big(\sqrt{Q^+}S|\Phi^-)(\Phi^-|S^*\sqrt{Q^+}\Big). \tag{5.76}$$

In particular, let $Q^+ = |\Phi^+)(\Phi^+|$. The matrix element

$$A = \left(\Phi^+|S\Phi^-\right)$$

is called a *scattering amplitude*. The corresponding transition probability equals

$$|A|^2 = \left|\left(\Phi^+|S\Phi^-\right)\right|^2.$$

Basic formalism of the scattering theory does not distinguish between the future and the past. (This is independent of whether there exists a time reversal symmetry or not). However, in practical applications of scattering theory, the difference between the past and the future is important.

(i) The initial state can be assumed to be very simple. In particular, in practice it involves one or two particles. One can suppose that it is prepared quite precisely, so that it is possible to describe it by a pure state.

(ii) On the other hand, the final state can be complicated and involve many particles. It is less natural to assume that it is given by a 1-dimensional projection. Typically, one considers a measurement of a spectral projection of a certain natural observable.

The observables that one would like to use to prepare and measure states, such as the *Hamiltonian* and the *momentum*, often have continuous spectrum, therefore they do not have normalizable eigenvectors. In order to obtain physically meaningful quantities, one needs to deal with their non-normalizable eigenvectors. We present typical heuristic arguments which are employed in this context in standard textbooks.

5.2 The square of the delta function

It is well known that the *square of Dirac's delta* is ill defined. However, when computing transition probabilities such an object appears naturally.

Suppose we assume that the process takes place within the time interval $[-T/2, T/2]$. Let E have the meaning of the energy, which is the dual variable to the time. In such a situation physics textbooks use the heuristic substitution

$$(2\pi\delta(E))^2 \ \to \ T2\pi\delta(E). \tag{5.77}$$

Similarly, suppose that the measurement takes place in a box of volume V, say, the cube $[-L/2, L/2]^d$ with $V = L^d$. Then we use the heuristic substitution

$$\big((2\pi)^d\delta(\vec{p})\big)^2 \ \to V(2\pi)^d\delta(\vec{p}). \tag{5.78}$$

One of heuristic justifications of (5.77) goes as follows. In the continuous case we have at our disposal integration

$$\int f(E)\mathrm{d}E \tag{5.79}$$

and the Dirac delta $\delta(E - E_1)$ which satisfies

$$\int \check{\delta}(E - E_1)f(E_1)\mathrm{d}E_1 = f(E). \tag{5.80}$$

Suppose that the system is time-periodic with the period T. Then the allowed values of the energy are $\frac{2\pi}{T}\mathbb{Z}$. Therefore, the integral (5.79) should be approximated by the Riemann sum

$$\sum_{E\in\frac{2\pi}{T}\mathbb{Z}} f(E)\frac{2\pi}{T}. \tag{5.81}$$

The Dirac delta $\delta(E)$ should be replaced by the appropriately normalized Kronecker delta $\check{\delta}_T(E_1 - E_2) := \frac{T}{2\pi}\check{\delta}_{E,E_1}$. Indeed, with this convention we have

$$\sum_{E_1\in\frac{2\pi}{T}\mathbb{Z}} \check{\delta}_T(E - E_1)f(E_1)\frac{2\pi}{T} = f(E), \tag{5.82}$$

which corresponds to the usual identity in the case of continuous energy (5.80).

Now,

$$\check{\delta}_T(E_1 - E_2)^2 = \frac{T}{2\pi}\check{\delta}_T(E_1 - E_2).$$

Another justification of (5.77) uses

$$\delta_T(E) := \frac{1}{2\pi}\int_{-T/2}^{T/2} \mathrm{d}t\mathrm{e}^{\mathrm{i}Et} = \frac{\sin ET/2}{\pi E}. \tag{5.83}$$

Note that

$$\int_{-\infty}^{\infty} \delta_T(E)\mathrm{d}E = 1 \tag{5.84}$$

hence δ_T is an approximate delta function. Moreover,

$$\int_{-\infty}^{\infty} \delta_T^2(E)\mathrm{d}E = \int_{-\infty}^{\infty} \frac{\sin^2 ET/2}{\pi^2 E^2}\mathrm{d}E = \frac{T}{2\pi}.$$

Hence $\frac{2\pi}{T}\delta_T^2$ is also an approximate delta function.

5.3 Measuring the energy

Suppose $I \subset \mathbb{R}$ is an interval of the energy that we want to measure. We also want to measure another independent observable, say, given by $\Pi^+ = |s^+)(s^+|$ Thus the operator describing our measured observable is

$$\mathbb{1}_I(H_0)\Pi^+ \approx \int_I \mathrm{d}E\frac{2\pi}{T}\delta_T^2(E - H_0)\Pi^+. \tag{5.85}$$

Thus if we prepare a state Φ^-, then the expectation value of the measurement of (5.85) is

$$(S\Phi^-|\mathbb{1}_I(H_0)\Pi^+ S\Phi^-) = \int_I \mathrm{d}E|(E, s^+|S\Phi^-)|^2 \tag{5.86}$$

$$\approx \int_I \mathrm{d}E\frac{2\pi}{T}(S\Phi^-|s^+)\delta_T(E - H_0)^2(s^+|S\Phi^-) \tag{5.87}$$

$$= \int_I \mathrm{d}E\frac{2\pi}{T}\|\delta_T(E - H_0)(s^+|S\Phi^-\|^2. \tag{5.88}$$

The measurement of the energy E and of Π^+ over time T can be represented by the application of the operator $\delta_T(H_0 - E)|s^+)(s^+|$. We have

$$\frac{T}{2\pi}|(E, s^+|S\Phi^-)|^2 \approx \|\delta_T(E - H_0)(s^+|S\Phi^-\|^2 \tag{5.89}$$

which is interpreted as the probability of measurement of energy E over time T.

Suppose that the theory is invariant wrt *time translations*. Then the scattering operator S commutes with the *free Hamiltonian* H_0. We can represent the Hilbert space as a *direct integral*

$$\mathcal{H} = \int^{\oplus} \mathcal{H}(E)\mathrm{d}E,$$

so that H_0 and S decompose:

$$H_0 = \int^{\oplus} E\mathrm{d}E, \quad S = \int^{\oplus} S(E)\mathrm{d}E.$$

Suppose that we consider the initial state

$$\Phi^- := \int f(E^-)|E^-, s^-)\mathrm{d}E^-.$$

Then (5.89) is

$$\frac{T}{2\pi}|(E, s^+|S(E)|E, s^-)|^2|f(E)|^2. \tag{5.90}$$

In the literature it is sometimes described heuristically as follows. We consider an initial state $|E^-, s^-) \in \mathcal{H}(E^-)$ and a final state $|E^+, s^+) \in \mathcal{H}(E^+)$. The corresponding *scattering amplitude* is given by

$$A(E^+, s^{(+)}; E^-, s^-) := \big(E^+, s^+|S(E^+)|E^-, s^-\big)\, \delta(E^+ - E^-).$$

The *transition probability* is the square of the scattering amplitude, where we take into account the heuristic formula for the square of the delta:

$$|A(E^+, s^+; E^-, s^-)|^2 = \big|\big(E^+, s^+|S(E^+)|E^-, e^-\big)\big|^2\, \frac{\delta(E^+ - E^-)T}{2\pi}.$$

The quantity of physical interest is the *transition probability per unit time*

$$\frac{|A(E^+, s^+; E^-, s^-)|^2}{T} = \big|\big(E^+, s^+|S(E^+)|E^-, s^-\big)\big|^2\, \frac{\delta(E^+ - E^-)}{2\pi}.$$

5.4 Measuring the momentum

This subsection is parallel to the previous one. Suppose that $\vec{P}$ is the momentum operator (generator of space translations). We want to measure the momentum inside $\Omega \subset \mathbb{R}^d$ together with an observable Π_{s^+}. We also want to measure another independent observable, say s^+ given by $\Pi_{s^+} = |s^+)(s^+|$ It corresponds to the observable

$$\mathbb{1}_\Omega(\vec{P})\Pi_{s^+} \approx \int_\Omega \frac{(2\pi)^d}{V}\delta_V^2(\vec{k} - \vec{P})\Pi_{s^+}, \tag{5.91}$$

where

$$\delta_V(\vec{k}) := \delta_L(k_1)\cdots\delta_L(k_d),$$

Thus if we prepare a state Φ^-, then the expectation value of the measurement of (5.91) is

$$(S\Phi^-|\mathbb{1}_\Omega(\vec{P})\Pi_{s_+}S\Phi^-) = \int_\Omega \mathrm{d}\vec{k}|(\vec{k},s^+|S\Phi^-)|^2 \tag{5.92}$$

$$\approx \int_\Omega \mathrm{d}\vec{k}\frac{(2\pi)^d}{V}\|\delta_V(\vec{P}-\vec{k})S\Phi^-\|^2, \tag{5.93}$$

Thus if we measure the momentum $\vec{P}=\vec{k}$ and Π_{s^+} in the volume $V=L^d$, which can be represented by the application of the operator $\delta_V(\vec{P}-\vec{k})\Pi_{s^+}$ on our state, we obtain the probability

$$\frac{V}{(2\pi)^d}|(\vec{k},s^+|S\Phi^-)|^2. \tag{5.94}$$

Suppose that the theory is invariant wrt *space translations*. Then the scattering operator S commutes with the *momentum* $\vec{P}$. We can represent the Hilbert space as a *direct integral* with respect to $\vec{k}$:

$$\mathcal{H} = \int^\oplus \mathcal{H}(\vec{k})\mathrm{d}\vec{k},$$

so that $\vec{P}$ and S decompose:

$$\vec{P} = \int^\oplus \vec{k}\mathrm{d}\vec{k}, \qquad S = \int^\oplus S(\vec{k})\mathrm{d}\vec{k}.$$

Suppose that we consider an initial and a final state $|\vec{k}^\pm,s^\pm) \in \mathcal{H}(\vec{k}^\pm)$. The scattering amplitudes are given by

$$A(\vec{k}^+,s^+;\vec{k}^-,s^-) := \left(\vec{k}^+,s^+|S(\vec{k}^+)|\vec{k}^-,s^-\right)\delta(\vec{k}^+-\vec{k}^-).$$

The transition probability is the square of the scattering amplitude:

$$|A(\vec{k}^+,s^+;\vec{k}^-,s^-)|^2 = \left|\left(\vec{k}^+,s^+)|S(\vec{k}^+)|\vec{k}^-,s^-\right)\right|^2\frac{\delta(\vec{k}^+-\vec{k}^-)V}{(2\pi)^d}.$$

The quantity of physical interest is the *transition probability per unit volume*

$$\frac{|A(\vec{k}^+,s^+;\vec{k}^-,s^-)|^2}{V} = \left|\left(\vec{k}^+,s^+|S(\vec{k}^+)|\vec{k}^-,s^-\right)\right|^2\frac{\delta(\vec{k}^+-\vec{k}^-)}{(2\pi)^d}.$$

5.5 Flux

We assume that $H_0(\vec{k},s| = E(\vec{k},s)(\vec{k},s|$ and $\vec{P}(\vec{k},s| = \vec{k}(\vec{k},s|$. Note that we have the normalization

$$\left(\vec{k},s|\vec{k}',s'\right) = \delta(\vec{k}-\vec{k}')\delta_{s,s'}.$$

Define the *velocity* by

$$\vec{v} = \nabla_{\vec{k}} E(\vec{k}, s).$$

In the relativistic case, when $E(\vec{k}) = \sqrt{m^2 + \vec{k}^2}$, we have

$$\vec{v} = \frac{\vec{k}}{E(\vec{k})}.$$

As an initial state we can take the plane wave restricted to the box $[-L/2, L/2]^d$. We set

$$\mathbb{1}_V(\vec{x}) := \mathbb{1}_{[-L/2,L/2]}(x_1) \cdots \mathbb{1}_{[-L/2,L/2]}(x_d),$$

$$|\vec{k}, s)_V := \frac{(2\pi)^{d/2}}{V^{1/2}} \mathbb{1}_V(\vec{x}) |\vec{k}, s) \tag{5.95}$$

$$= \frac{(2\pi)^{d/2}}{V^{1/2}} \int \cdots \int \delta_V(\vec{k}) \mathrm{d}\vec{k} |\vec{k}, s). \tag{5.96}$$

The amplitude is

$$\left(\Phi^+ | S | \vec{k^-}\right)_V$$

and the transition probability is

$$\left| \left(\Phi^+ | S | \vec{k^-}\right)_V \right|^2.$$

The *flux* is defined as $|\vec{v^-}| V^{-1}$. In applications one considers the *transition probability per unit flux*

$$\frac{\left| \left(\Phi^+ | S | \vec{k^-}\right)_V \right|^2}{|\vec{v^-}| V^{-1}}.$$

For $V \to \infty$ this converges to

$$\left| \left(\Phi^+ | S | \vec{k^-}\right) \right|^2 \frac{(2\pi)^d}{|\vec{v^-}|}.$$

Supose that the initial state describes a *pair of particles* described by the product of plane waves $|\vec{k_1^-}, \vec{k_2^-})$. Again, we use their finite volume version $|\vec{k_1^-}, \vec{k_2^-})_V$, obtaining the finite volume scattering amplitude

$$\left(\Phi^+ | S | \vec{k_1^-}, \vec{k_2^-}\right)_V.$$

As usual, the transition probability is

$$\left| \left(\Phi^+ | S | \vec{k_1^-}, \vec{k_2^-}\right)_V \right|^2.$$

First assume that $\vec{v_1^-}$ and $\vec{v_2^-}$ are *collinear*. Then the *flux for a pair of particles* is defined as $|\vec{v_1^-} - \vec{v_2^-}|V^{-2}$. The *transition probability per unit flux for a collinear pair of particles* equals

$$\frac{\left|\left(\Phi^+|S|\vec{k_1^-}, \vec{k_2^-}\right)_V\right|^2}{|\vec{v_1^-} - \vec{v_2^-}|V^{-2}}.$$

For $V \to \infty$ this converges to

$$\frac{\left|\left(\Phi^+|S|\vec{k_1^-}, \vec{k_2^-}\right)\right|^2 (2\pi)^{2d}}{|\vec{v_1^-} - \vec{v_2^-}|}.$$

In the relativistic case, for collinear $\vec{v_1^-}$ and $\vec{v_2^-}$ (and hence also for collinear $\vec{k_1^-}$ and $\vec{k_2^-}$), we have the identity

$$\frac{\sqrt{(k_1^- k_2^-)^2 - (m_1^-)^2 (m_2^-)^2}}{E_1^- E_2^-} = |\vec{v_1^-} - \vec{v_2^-}|.$$

Therefore, in the physics literature one defines *transition probability per unit flux for a pair of particles* by a Lorentz covariant expression

$$\left|\left(\Phi^+|S|\vec{k_1^-}, \vec{k_2^-}\right)\right|^2 \frac{(2\pi)^{2d} E_1^- E_2^-}{\sqrt{(k_1^- k_2^-)^2 - (m_1^-)^2 (m_2^-)^2}},$$

independently of whether the particle velocities are collinear or not.

6 Second quantization

In this chapter we describe the terminology and notation of multilinear algebra. We will concentrate on the infinite dimensional case, where it is often natural to use the structure of Hilbert spaces. We will introduce Fock spaces and various classes of operators acting on them. In quantum physics the passage from a dynamics on one-particle spaces to a dynamics on Fock spaces is often called *second quantization* – hence the name of the chapter.

6.1 Direct sum

Let $(\mathcal{Y}_i)_{i\in I}$ be a family of vector spaces. The *algebraic direct sum of* $\mathcal{Y}_i$ will be denoted

$$\overset{\text{al}}{\bigoplus_{i\in I}} \mathcal{Y}_i, \tag{6.97}$$

If $(\mathcal{Y}_i)_{i\in I}$ is a family of Hilbert spaces, then $\overset{\text{al}}{\bigoplus_{i\in I}} \mathcal{Y}_i$ has a natural scalar product. The *direct sum of* $\mathcal{Y}_i$ *in the sense of Hilbert spaces* is defined as

$$\bigoplus_{i\in I} \mathcal{Y}_i := \left(\overset{\text{al}}{\bigoplus_{i\in I}} \mathcal{Y}_i\right)^{\text{cpl}}.$$

If I is finite, then $\overset{\text{al}}{\oplus}_{i\in I} \mathcal{Y}_i = \oplus_{i\in I} \mathcal{Y}_i$

Let $(\mathcal{Y}_i)$, $(\mathcal{W}_i)$, $i \in I$, be families of vector spaces. If $a_i \in L(\mathcal{Y}_i, \mathcal{W}_i)$, $i \in I$, then their *direct sum* is denoted $\oplus_{i\in I} a_i$ and belongs to $L\left(\overset{\text{al}}{\oplus}_{i\in I} \mathcal{Y}_i, \overset{\text{al}}{\oplus}_{i\in I} \mathcal{W}_i\right)$.

Let $\mathcal{Y}_i$, $\mathcal{W}_i$, $i \in I$ be families of Hilbert spaces, and $a_i \in B(\mathcal{Y}_i, \mathcal{W}_i)$ with $\sup_{i\in I} \|a_i\| < \infty$. Then the operator $\oplus_{i\in I} a_i$ is bounded. Its extension in $B\left(\oplus_{i\in I} \mathcal{Y}_i, \oplus_{i\in I} \mathcal{W}_i\right)$ will be denoted by the same symbol.

6.2 Tensor product

Let $\mathcal{Y}, \mathcal{W}$ be vector spaces. The *algebraic tensor product of $\mathcal{Y}$ and $\mathcal{W}$* will be denoted $\mathcal{Y} \overset{\text{al}}{\otimes} \mathcal{W}$.

If $\mathcal{Y}$, $\mathcal{W}$ are Hilbert spaces, then $\mathcal{Y} \overset{\text{al}}{\otimes} \mathcal{W}$ has a unique scalar product such that

$$(y_1 \otimes w_1 | y_2 \otimes w_2) := (y_1|y_2)(w_1|w_2), \quad y_1, y_2 \in \mathcal{Y}, \quad w_1, w_2 \in \mathcal{W}.$$

We set

$$\mathcal{Y} \otimes \mathcal{W} := (\mathcal{Y} \overset{\text{al}}{\otimes} \mathcal{W})^{\text{cpl}},$$

and call it the *tensor product of $\mathcal{Y}$ and $\mathcal{W}$ in the sense of Hilbert spaces.*

If one of the spaces $\mathcal{Y}$ or $\mathcal{W}$ is finite dimensional, then $\mathcal{Y} \overset{\text{al}}{\otimes} \mathcal{W} = \mathcal{Y} \otimes \mathcal{W}$.

Let $\mathcal{Y}_1, \mathcal{Y}_2, \mathcal{W}_1, \mathcal{W}_2$ be vector spaces. If $a \in L(\mathcal{Y}_1, \mathcal{Y}_2)$ and $b \in L(\mathcal{W}_1, \mathcal{W}_2)$, then $a \otimes b$ denotes the *tensor product of a and b*, which is an operator in $L(\mathcal{Y}_1 \overset{\text{al}}{\otimes} \mathcal{W}_1, \mathcal{Y}_2 \overset{\text{al}}{\otimes} \mathcal{W}_2)$

If $\mathcal{Y}_1, \mathcal{Y}_2, \mathcal{W}_1, \mathcal{W}_2$ are Hilbert spaces and $a \in B(\mathcal{Y}_1, \mathcal{Y}_2)$, $b \in B(\mathcal{W}_1, \mathcal{W}_2)$, then $a \otimes b$ is bounded. It extends uniquely to an operator in $B(\mathcal{Y}_1 \otimes \mathcal{W}_1, \mathcal{Y}_2 \otimes \mathcal{W}_2)$, denoted by the same symbol.

To prove the boundedness of $a \otimes b$, it is sufficient to consider the operator $a \otimes \mathbb{1}$ from $\mathcal{Y}_1 \overset{\text{al}}{\otimes} \mathcal{W}$ to $\mathcal{Y}_2 \overset{\text{al}}{\otimes} \mathcal{W}$. Let $e_1, e_2, \dots$ and $f_1, f_2 \dots$ be orthonormal bases in $\mathcal{Y}_1$, $\mathcal{W}$ resp. Consider a vector $\sum c_{ij} \mathrm{e}_i \otimes f_j$.

$$\begin{aligned} \|a \otimes \mathbb{1} \sum c_{ij} e_i \otimes f_j\|^2 &= \sum_j \| \sum_i c_{ij} a e_i\|^2 \\ &\le \sum_j \|a\|^2 \sum_i |c_{ij}|^2 \\ &= \|a\|^2 \| \sum c_{ij} e_i \otimes f_j\|^2. \end{aligned}$$

6.3 Fock spaces

Let $\mathcal{Y}$ be a vector space. Let S_n denote the *permutation group of n elements* and $\sigma \in S_n$. $\Theta(\sigma)$ is defined as the unique operator in $L(\overset{\text{al}}{\otimes}^n \mathcal{Y})$ such that

$$\Theta(\sigma) y_1 \otimes \cdots \otimes y_n = y_{\sigma^{-1}(1)} \otimes \cdots \otimes y_{\sigma^{-1}(n)}.$$

We define the *symmetrization/antisymmetrization projections*

$$\Theta^n_{\rm s} := \frac{1}{n!}\sum_{\sigma\in S_n}\Theta(\sigma), \qquad \Theta^n_{\rm a} := \frac{1}{n!}\sum_{\sigma\in S_n}{\rm sgn}\sigma\Theta(\sigma).$$

If $\mathcal{Y}$ is a Hilbert space, then $\Theta(\sigma)$ is unitary and $\Theta^n_{\rm s/a}$ are orthogonal projections.

Let $\mathcal{Y}$ be a vector space. The *algebraic n-particle bosonic/fermionic space* is defined as

$$\overset{\rm al}{\otimes}{}^n_{\rm s/a}\mathcal{Y} := \Theta^n_{\rm s/a}\overset{\rm al}{\otimes}{}^n\mathcal{Y}.$$

The *algebraic bosonic/fermionic Fock space* or the *symmetric/antisymmetric tensor algebra* is

$$\overset{\rm al}{\Gamma}_{\rm s/a}(\mathcal{Y}) := \overset{\infty}{\underset{n=0}{\oplus}}\overset{\rm al}{\otimes}{}^n_{\rm s/a}\mathcal{Y}.$$

The *vacuum vector* is $\Omega := 1 \in \otimes^0_{\rm s/a}\mathcal{Y} = \mathbb{C}$.

If $\mathcal{Y}$ is a Hilbert space, then the *n-particle bosonic/fermionic space* is defined as

$$\otimes^n_{\rm s/a}\mathcal{Y} := \Theta^n_{\rm s/a}\otimes^n\mathcal{Y}.$$

The *bosonic/fermionic Fock space* is

$$\Gamma_{\rm s/a}(\mathcal{Y}) := \overset{\infty}{\underset{n=0}{\oplus}}\otimes^n_{\rm s/a}\mathcal{Y}.$$

For $z\in\mathcal{Y}$ we define the *creation operator*

$$\hat{a}^*(z)\Psi := \Theta^{n+1}_{\rm s/a}\sqrt{n+1}z\otimes\Psi, \quad \Psi\in\otimes^n_{\rm s/a}\mathcal{Y},$$

and the *annihilation operator* $\hat{a}(z) := (\hat{a}^*(z))^*$.

Above we used the *compact notation* for creation/annihilation operators popular among mathematicians. Physicists commonly prefer the *traditional notation*, which is longer and less canonical. In order to introduce it, we need to fix an identification of $\mathcal{Y}$ with $L^2(\Xi)$ for some measure space $(\Xi,{\rm d}\xi)$. If z equals a function $\Xi\ni\xi\mapsto z(\xi)$, then

$$\hat{a}^*(z) = \int z(\xi)\hat{a}^*_\xi{\rm d}\xi, \quad \hat{a}(z) = \int \overline{z}(\xi)\hat{a}_\xi{\rm d}\xi.$$

6.4 Second quantization of operators

For a contraction q on $\mathcal{Z}$ we define the operator $\Gamma(q)$ on $\Gamma_{\rm s/a}(\mathcal{Z})$ by

$$\Gamma(q)\Big|_{\otimes^n_{\rm s/a}\mathcal{Z}} = q\otimes\cdots\otimes q\Big|_{\otimes^n_{\rm s/a}\mathcal{Z}}.$$

$\Gamma(q)$ is called the *second quantization of* q.

Similarly, for an operator h we define the operator $\mathrm{d}\Gamma(h)$ by

$$\mathrm{d}\Gamma(h)\Big|_{\otimes^n_{\mathrm{s/a}}\mathcal{Z}} = h\otimes 1^{(n-1)\otimes} + \cdots + 1^{(n-1)\otimes}\otimes h\Big|_{\otimes^n_{\mathrm{s/a}}\mathcal{Z}}.$$

$\mathrm{d}\Gamma(h)$ is called the *(infinitesimal) second quantization of* h.

Traditional notation: If h is the multiplication operator by $h(\xi)$, then $\mathrm{d}\Gamma(h) = \int h(\xi)a^*_\xi a_\xi \mathrm{d}\xi$. This will be justified in (6.104).

Note the identity $\Gamma(\mathrm{e}^{\mathrm{i}th}) = \mathrm{e}^{\mathrm{i}t\mathrm{d}\Gamma(h)}$.

6.5 Wick quantization

Let

$$(\xi_1,\cdots\xi_m,\xi'_k,\cdots,\xi'_1)\mapsto b(\xi_1,\cdots\xi_m,\xi'_k,\cdots,\xi'_1) \tag{6.98}$$

be a complex function, symmetric/antisymmetric separately wrt the first m and the last k arguments. It can be treated as the kernel of a *symmetric/antisymmetric multilinear function* on $\overline{\mathcal{Z}}\oplus\mathcal{Z}$:

$$\int\cdots\int b(\xi_1,\cdots\xi_m,\xi'_k,\cdots,\xi'_1)$$
$$\overline{a(\xi_1)}\cdots\overline{a(\xi_m)}a(\xi'_k)\cdots a(\xi'_1)\mathrm{d}\xi_1\cdots\mathrm{d}\xi_m\mathrm{d}\xi'_k\cdots\mathrm{d}\xi'_1.$$

In the symmetric case this can be interpreted as a *polynomial on* $\mathcal{Z}$. It is common to use the name a *polynomial* also in the antisymmetric case.

Note that (6.98) can be also interpreted as the integral kernel of an *operator* from $\otimes^k_{\mathrm{s/a}}\mathcal{Z}$ to $\otimes^m_{\mathrm{s/a}}\mathcal{Z}$.

The *Wick quantization of the polynomial* b will have two notations: the compact and the traditional:

$$\begin{aligned} b(\hat a^*,\hat a) &= \int b(\xi_1,\cdots\xi_m,\xi'_k,\cdots,\xi'_1) \\ &\quad \hat a^*(\xi_1)\cdots\hat a^*(\xi_m)\hat a(\xi'_k)\cdots\hat a(\xi'_1)\mathrm{d}\xi_1,\cdots\mathrm{d}\xi_k\mathrm{d}\xi'_1\cdots\mathrm{d}\xi'_m. \end{aligned} \tag{6.99}$$

Its only nonzero matrix elements are between $\Phi\in\otimes^{p+m}_{\mathrm{s/a}}\mathcal{Z}$, $\Psi\in\otimes^{p+k}_{\mathrm{s/a}}\mathcal{Z}$, and equal

$$(\Phi|b(\hat a^*,\hat a)\Psi) = \frac{\sqrt{(m+p)!(k+p)!}}{p!}(\Phi|b\otimes 1^{\otimes p}_{\mathcal{Z}}\Psi). \tag{6.100}$$

Actually, we can also consider b which is not symmetric/antisymmetric. The operator (6.99) defined by such b will depend only on its symmetrization/antisymmetrization. In particular, if b is interpreted as an operator from $\otimes^k\mathcal{Z}$ to $\otimes^m\mathcal{Z}$, then

$$b(a^*,a) = b^{\mathrm{s/a}}(a^*,a),\quad b^{\mathrm{s/a}} := \Theta^m_{\mathrm{s/a}}b\Theta^k_{\mathrm{s/a}}.$$

6.6 Particle number preserving operators

If $m = k$, then the operator $b(\hat{a}^*, \hat{a})$ preserves the number of particles and (6.100). For $\Phi \in \otimes^n_{\mathrm{s/a}} \mathcal{Z}$, $\Psi \in \otimes^n_{\mathrm{s/a}} \mathcal{Z}$ it can be rewritten as

$$(\Phi | b(\hat{a}^*, \hat{a}) \Psi) \quad = \quad \frac{n!}{(n-m)!} (\Phi | b \otimes 1_{\mathcal{Z}}^{\otimes(n-m)} \Psi). \tag{6.101}$$

But $\frac{n!}{(n-m)!m!}$ is the number of m-element subsets of $\{1, 2, \ldots, n\}$. Therefore, we can rewrite, in the obvious notation, (6.101) as

$$\frac{1}{m!} b(\hat{a}^*, \hat{a}) = \sum_{1 \leq i_1 < \cdots < i_m \leq n} b_{i_1, \ldots, i_m}. \tag{6.102}$$

In particular, for $m = 2$ we can write

$$\frac{1}{2} b(\hat{a}^*, \hat{a}) = \sum_{1 \leq i < j \leq n} b_{ij}. \tag{6.103}$$

Finally, for $m = 1$, we have

$$b(\hat{a}^*, \hat{a}) = \sum_{1 \leq i \leq n} b_i = \mathrm{d}\Gamma(b). \tag{6.104}$$

6.7 Examples

Consider $L^2(\mathbb{R}^d)$. We have the position representation, with the generic variables x, y and the momentum representation with the generic variables k, k'. We can pass from one representation to the other by

$$a^*(k) = (2\pi)^{-\frac{d}{2}} \int a^*(x) \mathrm{e}^{-\mathrm{i}kx} \mathrm{d}x, \quad a^*(x) = (2\pi)^{-\frac{d}{2}} \int a^*(k) \mathrm{e}^{\mathrm{i}kx} \mathrm{d}k, \tag{6.105}$$

$$a(k) = (2\pi)^{-\frac{d}{2}} \int a(x) \mathrm{e}^{\mathrm{i}kx} \mathrm{d}x, \qquad a(x) = (2\pi)^{-\frac{d}{2}} \int a(k) \mathrm{e}^{-\mathrm{i}kx} \mathrm{d}k. \tag{6.106}$$

Here we give a few quadratic operators in the two representations:

$$\mathrm{d}\Gamma(h) \; = \int\int a^*(x) h(x,y) a(y) \mathrm{d}x \mathrm{d}y = (2\pi)^{-d} \int\int a^*(k) \hat{h}(-k, k') a(k') \mathrm{d}k \mathrm{d}k',$$

$$\text{where } \hat{h}(k, k') := \int\int h(x,y) \mathrm{e}^{-\mathrm{i}kx - \mathrm{i}k'y} \mathrm{d}x \mathrm{d}y;$$

$$\mathrm{d}\Gamma(V(x)) \; = \; \int a^*(x) V(x) a(x) \mathrm{d}x = (2\pi)^{-d} \int a^*(k) \hat{V}(-k + k') a(k') \mathrm{d}k \mathrm{d}k'$$

$$\text{where } \hat{V}(k) := \int V(x) \mathrm{e}^{-\mathrm{i}kx} \mathrm{d}x;$$

$$\mathrm{d}\Gamma(-\Delta) \; = \; \int a^*(x) (-\Delta_x) a(x) \mathrm{d}x = \int a^*(k) k^2 a(k) \mathrm{d}k.$$

Consider $L^2([0,L]^d) \simeq L^2\Big(\frac{2\pi}{L}\mathbb{Z}^d\Big)$. Again we use x, y in the position representation an k, k' in the momentum representation. We can pass from one representation to the other by

$$a^*(k) = L^{-\frac{d}{2}} \int a(x) \mathrm{e}^{-\mathrm{i}kx} \mathrm{d}x, \qquad a^*(x) = L^{-\frac{d}{2}} \sum_k a(k) \mathrm{e}^{\mathrm{i}kx}, \tag{6.107}$$

$$a(k) = L^{-\frac{d}{2}} \int a(x) \mathrm{e}^{\mathrm{i}kx} \mathrm{d}x, \qquad a(x) = L^{-\frac{d}{2}} \sum_k a(k) \mathrm{e}^{-\mathrm{i}kx}. \tag{6.108}$$

Here we give a few quadratic operators in the two representations:

$$\begin{aligned}
\mathrm{d}\Gamma(h) \ &= (2\pi)^{-d} \int\int a^*(x) h(x,y) a(y) \mathrm{d}x\mathrm{d}y = L^{-d} \sum_k \sum_{k'} a^*(k) \hat{h}(-k,k') a(k'), \\
&\qquad\qquad \text{where } \hat{h}(k,k') := \int\int h(x,y) \mathrm{e}^{-\mathrm{i}kx - \mathrm{i}k'y} \mathrm{d}x\mathrm{d}y; \\
\mathrm{d}\Gamma(V(x)) \ &= \int a^*(x) V(x) a(x) \mathrm{d}x = L^{-d} \sum_{k,k'} a^*(k) \hat{V}(-k+k') a(k') \\
&\qquad\qquad \text{where } \hat{V}(k) := \int V(x) \mathrm{e}^{-\mathrm{i}kx} \mathrm{d}x; \\
\mathrm{d}\Gamma(-\Delta) \ &= \int a^*(x) (-\Delta_x) a(x) \mathrm{d}x = \sum_k a^*(k) k^2 a(k).
\end{aligned}$$

Now consider the 2-body potential $V(x-y)$. Denote this operator by b. Its kernel in the position and momentum representation is

$$b(x,y;y',x') = V(x-y)\delta(x-x')\delta(y-y'), \tag{6.109}$$

$$b(k,p,p',k') = (2\pi)^{-d} \hat{V}(-p+p')\delta(p+k-p'-k'). \tag{6.110}$$

Indeed,

$$\begin{aligned}
&(p'|(q'|V(x-y)|p)|q) \\
=&(2\pi)^{-2d} \int\int \mathrm{e}^{-\mathrm{i}p'x} \mathrm{e}^{-\mathrm{i}q'y} \mathrm{e}^{\mathrm{i}px} \mathrm{e}^{\mathrm{i}qy} V(x-y) \mathrm{d}x\mathrm{d}y \\
&= (2\pi)^{-2d} \int\int \mathrm{e}^{\mathrm{i}(p-p')(x-y)} \mathrm{e}^{-\mathrm{i}y(p+q-p'-q')} V(x-y) \mathrm{d}x\mathrm{d}y \\
&= (2\pi)^{-d} \hat{V}(-p+p') \delta(p+q-p'-q').
\end{aligned}$$

Therefore,

$$\int\int \mathrm{d}x\mathrm{d}y V(x-y) a_x^* a_y^* a_y a_x = (2\pi)^{-d} \int\int\int \mathrm{d}p\mathrm{d}q\mathrm{d}k \hat{V}(k) a_{p+k}^* a_{q-k}^* a_q a_p.$$

Similarly, in the box we have

$$\int\int \mathrm{d}x\mathrm{d}y V(x-y) a_x^* a_y^* a_y a_x = L^{-d} \sum_p \sum_q \sum_k \hat{V}(k) a_{p+k}^* a_{q-k}^* a_q a_p.$$

For example, consider the Schrödinger Hamiltonian of n identical particles

$$H_n = -\sum_{i=1}^{n} \Delta_i + \sum_{1\le i<j\le n} V(x_i - x_j), \tag{6.111}$$

$$P_n = \sum_{i=1}^{n} \frac{1}{\mathrm{i}} \partial_{x_i}, \tag{6.112}$$

In the momentum representation

$$\begin{aligned} H_n &= \sum_{i=1}^{n} \int p^2 |p)_i (p|_i \mathrm{d}p \\ &\quad + (2\pi)^{-d} \sum_{1\le i<j\le N} \int \delta(p' + q' - q - \mathrm{p}) \hat{V}(p' - p) |p')_i |q')_j (q|_j (\mathrm{p}|_i. \\ P_n &= -\sum_{i=1}^{n} \int p|p)_i (p|_i \mathrm{d}p. \end{aligned}$$

In the 2nd quantized notation we can rewrite all this as

$$\begin{aligned} H := \bigoplus_{n=0}^{\infty} H_n &= -\int a_x^* \Delta_x a_x \mathrm{d}x \\ &\quad + \int\int \mathrm{dxd}y V(x-y) a_x^* a_y^* a_y a_x \\ &= \int p^2 a_p^* a_p \mathrm{d}p \\ &\quad + (2\pi)^{-d} \int\int\int \mathrm{dpd}q\mathrm{d}k \hat{V}(k) a_{p+k}^* a_{q-k}^* a_q a_p \\ P := \bigoplus_{n=0}^{\infty} P_n &= \int a_x^* \frac{1}{\mathrm{i}} \partial_x a_x \mathrm{d}x \\ &= \int p a_p^* a_p \mathrm{d}p. \end{aligned}$$

7 Coherent states and van Hove Hamiltonians

7.1 Translation in phase space

The *Baker-Campbell-Hausdorff formula* says that if $[A,[A,B]] = [B,[A,B]] = 0$, then

$$\mathrm{e}^{A+B} = \mathrm{e}^{A} \mathrm{e}^{B} \mathrm{e}^{-\frac{1}{2}[A,B]}.$$

In particular, consider a Hilbert space $L^2(\Xi, \mathrm{d}\xi)$ and the corresponding Fock space $\Gamma_{\mathrm{s}}(L^2(\Xi, \mathrm{d}\xi))$. Let $g \in L^2(\Xi)$.

$$\mathrm{e}^{a^*(g) - a(g)} = \mathrm{e}^{-\frac{1}{2}(g|g)} \mathrm{e}^{a^*(g)} \mathrm{e}^{-a(g)}.$$

We have

$$\mathrm{e}^{-a^*(g)+a(g)}a(\xi)\mathrm{e}^{a^*(g)-a(g)} = a(\xi) + g(\xi), \tag{7.113}$$

$$\mathrm{e}^{-a^*(g)+a(g)}a^*(\xi)\mathrm{e}^{a^*(g)-a(g)} = a^*(\xi) + \overline{g(\xi)}. \tag{7.114}$$

7.2 Coherent vectors

$$\Omega_g := \mathrm{e}^{a^*(g)-a(g)}\Omega = \mathrm{e}^{-\frac{1}{2}(g|g)}\mathrm{e}^{a^*(g)}\Omega.$$

is called a coherent vector associated to g.

Suppose $H = h(a^*, a)$ is a Hamiltonian. Then we can easily compute the expectation value of H in Ω_g:

$$(\Omega_g|H\Omega_g) = (\Omega|\mathrm{e}^{-a^*(g)+a(g)}h(a^*, a)\mathrm{e}^{a^*(g)-a(g)}\Omega)$$
$$= (\Omega|h(a^* + g, a + \overline{g})\Omega) = h(g, \overline{g}).$$

Therefore,

$$\inf H \leq \inf h.$$

Another point of view: We introduce

$$b(\xi) := a(\xi) - g(\xi), \quad b^*(\xi) := a^*(\xi) - \overline{g(\xi)}.$$

Then b^*, b satisfy the same commutation relations as a^*, a. Ω_g is a new "vacuum:

$$b(\xi)\Omega_g = 0.$$

We use b^*, b instead of a^*, a, in particular $H = h(b^* + g, b + \overline{g})$.

This is just an equivalent approach if g is square integrable, since the two points of view are unitarily equivalent. However, this is often used when g is not square integrable–then we use a different representation of CCR. The "classical Hamiltonian" is the same, however the "quantum representation" has been changed.

7.3 Van Hove Hamiltonians

Let $\xi \mapsto \omega(\xi) \geq 0$. Consider the self-adjoint operator $H_0 = \int \omega(\xi)a^*(\xi)a(\xi)\mathrm{d}\xi$ and the perturbation $V = \int v(\xi)a^*(\xi)\mathrm{d}\xi + \int \overline{v(\xi)}a(\xi)\mathrm{d}\xi$.
The operator given by $H := H_0 + V$ will be called a *van Hove Hamiltonian*.

Van Hove Hamiltonians are exactly solvable. Nevertheless, their theory is surprisingly rich. To avoid the *ultraviolet problem* we will always assume

$$\int_{\omega\geq 1} |v(\xi)|^2\mathrm{d}\xi < \infty.$$

We will discuss various possible infra-red behaviors of van Hove Hamiltonians.

Formally, we can write

$$H = \int \omega(\xi)\Big(a^*(\xi) + \frac{\overline{v(\xi)}}{\omega(\xi)}\Big)\Big(a(\xi) + \frac{v(\xi)}{\omega(\xi)}\Big)\mathrm{d}\xi - \int \frac{|v(\xi)|^2}{\omega(\xi)}\mathrm{d}\xi. \tag{7.115}$$

Infrared case A.

$$\int_{\omega<1} \frac{|v(\xi)|^2}{\omega(\xi)^2} \mathrm{d}\xi \quad < \quad \infty.$$

Introduce the *dressing operator*

$$\begin{aligned} U &:= \exp\left(-\int \frac{v(\xi)}{\omega(\xi)} a^*(\xi)\mathrm{d}\xi + \int \frac{\overline{v(\xi)}}{\omega(\xi)} a(\xi)\mathrm{d}\xi\right) \\ &= \exp\left(-\int \frac{v(\xi)}{\omega(\xi)} a^*(\xi)\mathrm{d}\xi\right) \exp\left(\int \frac{\overline{v(\xi)}}{\omega(\xi)} a(\xi)\mathrm{d}\xi\right) \\ &\quad \times \exp\left(-\frac{1}{2}\int \frac{|v(\xi)|^2}{\omega(\xi)^2}\mathrm{d}\xi\right) \end{aligned}$$

and the *ground state energy*

$$E := -\int \frac{|v(\xi)|^2}{\omega(\xi)}\mathrm{d}\xi.$$

The operator H is well defined and, up to a constant, is unitarily equivalent to H_0:

$$H - E = U H_0 U^*$$

Clearly, the Fock vacuum $\Phi_0 = \Omega$ is the unique ground state of H_0 with the eigenvalue $E_0 = 0$. Therefore H has a unique ground state

$$\Psi = \exp\left(-\int \frac{|v(\xi)|^2}{2\omega(\xi)^2}\mathrm{d}\xi\right) \exp\left(-\int a^*(\xi)\frac{v(\xi)}{\omega(\xi)}\mathrm{d}\xi\right)\Omega,$$

and its eigenvalue is E.

Infrared case B

Let

$$\begin{aligned} \int_{\omega<1} \frac{|v(\xi)|^2}{\omega(\xi)}\mathrm{d}\xi &< \infty; \\ \int_{\omega<1} \frac{|v(\xi)|^2}{\omega(\xi)^2}\mathrm{d}\xi &= \infty. \end{aligned}$$

Then H is well defined, has the spectrum $[E, \infty[$, but has no bound states.

Infrared case C.

Let

$$\begin{aligned} \int_{\omega<1} |v(\xi)|^2\mathrm{d}\xi &< \infty; \\ \int_{\omega<1} \frac{|v(\xi)|^2}{\omega(\xi)}\mathrm{d}\xi &= \infty. \end{aligned}$$

Then H is well defined, but $\mathrm{sp}H =]-\infty, \infty[$.

7.4 Dynamics of time-independent van Hove Hamiltonians

It is easy to compute $\mathrm{e}^{\mathrm{i}tH}$ in the case A:

$$\begin{aligned}
\mathrm{e}^{\mathrm{i}tH} &= \exp\Big(-a^*\big(\omega^{-1}v\big)+a\big(\omega^{-1}v\big)\Big)\Gamma\big(\mathrm{e}^{\mathrm{i}t\omega}\big)\exp\Big(a^*\big(\omega^{-1}v\big)-a\big(\omega^{-1}v\big)\Big)\\
&\quad\times\exp\Big(-\mathrm{i}t(v|\omega^{-1}v)\Big)\\
&= \exp\Big(-a^*\big(\omega^{-1}v\big)+a\big(\omega^{-1}v\big)\Big)\exp\Big(a^*\big(\mathrm{e}^{\mathrm{i}t\omega}\omega^{-1}v\big)-a\big(\mathrm{e}^{\mathrm{i}t\omega}\omega^{-1}v\big)\Big)\\
&\quad\times\Gamma\big(\mathrm{e}^{\mathrm{i}t\omega}\big)\exp\Big(-\mathrm{i}t(v|\omega^{-1}v)\Big)\\
&= \exp\Big(a^*\big((\mathrm{e}^{\mathrm{i}t\omega}-1)\omega^{-1}v\big)+a\big((1-\mathrm{e}^{\mathrm{i}t\omega})\omega^{-1}v\big)\Big)\\
&\quad\times\Gamma\big(\mathrm{e}^{\mathrm{i}t\omega}\big)\exp\Big(\frac{1}{2}\big(v|(\mathrm{e}^{\mathrm{i}t\omega}-\mathrm{e}^{-\mathrm{i}t\omega}-\mathrm{i}2t\omega)\omega^{-2}v\big)\Big).
\end{aligned}$$

We easily see that the above expression is well defined in the case A, B and C for all t and strongly continuously depends on t. Therefore, H is well defined as a self-adjoint operator.

7.5 Reminder about notation for evolution

It is convenient to use the following notation for a dynamics generated by time dependent Hamiltonian $H(t)$:

$$U(t_+,t_-) := \mathrm{Texp}\left(-\mathrm{i}\int_{t_-}^{t_+} H(s)\mathrm{d}s\right).$$

The *evolution in the interaction picture* is defined as

$$U_{\mathrm{Int}}(t_+,t_-) \;:=\; \mathrm{e}^{\mathrm{i}t_+H_0}U(t_+,t_-)\mathrm{e}^{-\mathrm{i}t_-H_0}.$$

The *interaction Hamiltonian* is defined as

$$H_{\mathrm{Int}}(t) := \mathrm{e}^{\mathrm{i}tH_0}V(t)\mathrm{e}^{-\mathrm{i}tH_0}.$$

Note that

$$U_{\mathrm{Int}}(t_+,t_-) \;=\; \mathrm{Texp}\left(-\mathrm{i}\int_{t_-}^{t_+} H_{\mathrm{Int}}(t)\mathrm{d}t\right).$$

$$S^{\pm} := U_{\mathrm{Int}}(0,\pm\infty)$$

are called *Møller operators* and

$$S := U_{\mathrm{Int}}(\infty,-\infty)$$

is called the scattering operator.

7.6 Time-dependent BCH formula

Let $\mathbb{R} \ni t \mapsto A(t), B(t)$ be operator valued functions such that

$$[A(t), A(t')] = [B(t), B(t')] = 0,$$

$$[[A(t), B(t')], A(t'')] = [[A(t), B(t')], B(t'')] = 0.$$

Then

$$\mathrm{Texp}\left(\int_{-\infty}^{\infty} \mathrm{d}t(A(t) + B(t))\right) \tag{7.116}$$

$$= \exp\left(\int_{-\infty}^{\infty} \mathrm{d}tA(t)\right) \exp\left(\int_{-\infty}^{\infty} \mathrm{d}tB(t)\right) \tag{7.117}$$

$$\times \exp\left(\int_{-\infty}^{\infty} \mathrm{d}t_1 \int_{-\infty}^{\infty} \mathrm{d}t_2 \theta(t_1 - t_2)[B(t_1), A(t_2)]\right). \tag{7.118}$$

The exponent of (7.118) by a simple substitution can be rewritten as

$$\int_{-\infty}^{\infty} \mathrm{d}t_1 \int_{-\infty}^{\infty} \mathrm{d}t_2 \theta(t_1 - t_2)[B(t_1), A(t_2)] \tag{7.119}$$

$$= \frac{1}{2} \int_{-\infty}^{\infty} \mathrm{d}t_1 \int_{-\infty}^{\infty} \mathrm{d}t_2 \Big(\theta(t_1 - t_2)[B(t_1), A(t_2)] + \theta(t_2 - t_1)[B(t_2), A(t_1)]\Big).$$

7.7 Time dependent Van Hove Hamiltonians

The BCH formula has the following time-dependent version:

Consider a *(time-dependent) Van Hove Hamiltonian* $H(t) := H_0 + V(t)$ with

$$V(t) = \int v(t, \xi) a^*(\xi) \mathrm{d}\xi + \int \overline{v(t, \xi)} a(\xi) \mathrm{d}\xi.$$

Clearly, the van Hove Hamiltonian in the interaction picture equals

$$H_{\mathrm{Int}}(t) = \int \mathrm{e}^{\mathrm{i}t\omega(\xi)} v(t, \xi) a^*(\xi) \mathrm{d}\xi + \int \mathrm{e}^{-\mathrm{i}t\omega(\xi)} \overline{v(t, \xi)} a(\xi) \mathrm{d}\xi.$$

Theorem 7.1 *The corresponding scattering operator is then given by*

$$\begin{aligned} S &= \mathrm{Texp}\left(-\mathrm{i} \int H_{\mathrm{Int}}(t) \mathrm{d}t\right) \\ &= \exp\left(-\mathrm{i} \int v(\omega(\xi), \xi) a^*(\xi) \mathrm{d}\xi\right) \exp\left(-\mathrm{i} \int \overline{v(\omega(\xi), \xi)} a(\xi) \mathrm{d}\xi\right) \\ &\quad \times \exp\left(\frac{\mathrm{i}}{2\pi} \int \frac{\overline{v(\tau, \xi)} v(\tau, \xi) \omega(\xi)}{\omega(\xi)^2 - \tau^2 - \mathrm{i}0} \mathrm{d}\tau \mathrm{d}\xi\right), \end{aligned}$$

where $v(\tau, \xi) := \int v(t, \xi) \mathrm{e}^{\mathrm{i}t\tau} \mathrm{d}t$.

Proof. We apply the time-dependent BCH formula with

$$A(t) := -\mathrm{i}\int \mathrm{e}^{\mathrm{i}t\omega(\xi)} v(t,\xi) a^*(\xi)\mathrm{d}\xi, \tag{7.120}$$

$$B(t) := -\mathrm{i}\int \mathrm{e}^{-\mathrm{i}t\omega(\xi)} \overline{v(t,\xi)} a(\xi)\mathrm{d}\xi. \tag{7.121}$$

We obtain

$$S = \exp\left(-\mathrm{i}\int \mathrm{d}\xi \int \mathrm{d}t \mathrm{e}^{\mathrm{i}t\omega(\xi)} v(t,\xi) a^*(\xi)\right) \exp\left(-\mathrm{i}\int \mathrm{d}\xi \int \mathrm{d}t \mathrm{e}^{-\mathrm{i}t\omega(\xi)} \overline{v(t,\xi)} a(\xi)\right)$$
$$\times \exp\left(-\frac{1}{2}\int \mathrm{d}\xi \int \mathrm{d}t_1 \int \mathrm{d}t_2 \mathrm{e}^{-\mathrm{i}\omega(\xi)|t_1-t_2|} \overline{v(t_1,\xi)} v(t_2,\xi)\right).$$

□

Let us note the identity

$$-\frac{1}{2}\int\int \mathrm{d}t_1 \mathrm{d}t_2 \Big(\Omega|\mathrm{T}\big(H_{\mathrm{Int}}(t_1) H_{\mathrm{Int}}(t_2)\big)\Omega\Big) \tag{7.122}$$

$$= -\frac{1}{2}\int \mathrm{d}\xi \int \mathrm{d}t_1 \int \mathrm{d}t_2 \mathrm{e}^{-\mathrm{i}\omega(\xi)|t_1-t_2|} \overline{v(t_1,\xi)} v(t_2,\xi) \tag{7.123}$$

$$= \frac{\mathrm{i}}{2\pi}\int \frac{\overline{v(\tau,\xi)} v(\tau,\xi)\omega(\xi)}{\omega(\xi)^2 - \tau^2 - \mathrm{i}0}\mathrm{d}\tau\mathrm{d}\xi, \tag{7.124}$$

which shows that a kind of a Feynman propagator appears naturally in this context.

7.8 Adiabatic scattering theory for van Hove Hamiltonians

Assume for the moment that H_0, V be self-adjoint operators and $\epsilon > 0$. We define $V_\epsilon(t) := \mathrm{e}^{-\epsilon|t|} V$. We will write

$$H_\epsilon(t) := H_0 + V_\epsilon$$

for the corresponding time-dependent Hamiltonian. We also introduce $U_\epsilon(t_+, t_-)$, $U_{\epsilon\mathrm{Int}}(t_+, t_-)$, $S_\epsilon^\pm$, S_ϵ, etc.

We can compute the *adiabatic Møller operator* for van Hove Hamiltonians. To this end, consider $v_\epsilon^+(t,\xi) := \theta(t)\mathrm{e}^{-\epsilon|t|} v(\xi)$. Then $v_\epsilon^+(\tau,\xi) = \frac{\mathrm{i}v(\xi)}{\tau+\mathrm{i}\epsilon}$. We have

$$\begin{aligned} S_\epsilon^+ \;=\; & \exp\left(\int \frac{v(\xi)}{\omega(\xi)+\mathrm{i}\epsilon} a^*(\xi)\mathrm{d}\xi\right) \exp\left(-\int \frac{\overline{v(\xi)}}{\omega(\xi)-\mathrm{i}\epsilon} a(\xi)\mathrm{d}\xi\right) \\ & \times \exp\left(\frac{\mathrm{i}}{2\pi}\int \frac{|v(\xi)|^2 \omega(\xi)\mathrm{d}\tau\mathrm{d}\xi}{(\tau^2+\epsilon^2)(\omega(\xi)^2-\tau^2-\mathrm{i}0)}\right). \end{aligned} \tag{7.125}$$

(7.125) does not have a limit as $\epsilon \searrow 0$. Indeed, an elementary calculation shows

$$\begin{aligned}\int \frac{\mathrm{d}\tau}{(\tau^2+\epsilon^2)(\omega(\xi)^2-\tau^2-\mathrm{i}0)} &= \int \frac{1}{\omega(\xi)^2+\epsilon^2}\left(\frac{1}{\tau^2+\epsilon^2}+\frac{1}{\omega(\xi)^2-\tau^2-\mathrm{i}0}\right)\mathrm{d}\tau \\ &= \frac{\pi}{\epsilon(\omega(\xi)^2+\epsilon^2)}+\frac{\mathrm{i}\pi}{\omega(\xi)(\omega(\xi)^2+\epsilon^2)}. \qquad (7.126)\end{aligned}$$

Now the real part of $\frac{\mathrm{i}\omega(\xi)}{2\pi}$(7.126) equals $-\frac{1}{2(\omega(\xi)^2+\epsilon^2)}$. Therefore we can renormalize S_ϵ by removing the divergent phase:

$$\begin{aligned}\frac{|(\Omega|S_\epsilon^+\Omega)|}{(\Omega|S_\epsilon^+\Omega)}S_\epsilon^+ &= \exp\left(-\int\frac{v(\xi)}{\omega(\xi)+\mathrm{i}\epsilon}a^*(\xi)\mathrm{d}\xi\right)\exp\left(\int\frac{\overline{v(\xi)}}{\omega(\xi)-\mathrm{i}\epsilon}a(\xi)\mathrm{d}\xi\right) \\ &\quad\times\exp\left(-\frac{1}{2}\int\frac{|v(\xi)|^2}{\omega(\xi)^2+\epsilon^2}\mathrm{d}\xi\right).\end{aligned}$$

Therefore, if $\int\frac{|v(\xi)|^2}{\omega(\xi)^2}\mathrm{d}\xi<\infty$, that is in Case A, then the *Gell-Mann and Low wave operator for H* equals

$$\begin{aligned}S_{\mathrm{GL}}^+ &= \mathrm{s}\text{-}\lim_{\epsilon\searrow 0}\frac{|(\Omega|S_\epsilon^+\Omega)|}{(\Omega|S_\epsilon^+\Omega)}S_\epsilon^+ \\ &= \exp\left(-\int\frac{v(\xi)}{\omega(\xi)}a^*(\xi)\mathrm{d}\xi\right)\exp\left(\int\frac{\overline{v(\xi)}}{\omega(\xi)}a(\xi)\mathrm{d}\xi\right) \\ &\quad\times\exp\left(-\frac{1}{2}\int\frac{|v(\xi)|^2}{\omega(\xi)^2}\mathrm{d}\xi\right)\end{aligned}$$

and coincides with the dressing operator U^*.

If $\int\frac{|v(\xi)|^2}{\omega(\xi)^2}\mathrm{d}\xi=\infty$, that is in Case B and C, then S_{GL}^+ does not exist because of the *infrared problem*.

An analogous computation yields $S_{\mathrm{GL}}^- = S_{\mathrm{GL}}^+$. Therefore, the *Gell-Mann and Low scattering operator for H* equals

$$S_{\mathrm{GL}} := S_{\mathrm{GL}}^{+*}S_{\mathrm{GL}}^- = \mathbb{1}.$$

One can also compute S_{GL} directly, setting $v(t,\xi) := \mathrm{e}^{-\epsilon|t|}v(\xi)$. Then $v(\tau,\xi)=\frac{2\epsilon}{\tau^2+\epsilon^2}v(\xi)$. Therefore,

$$\frac{S_\epsilon}{(\Omega|S_\epsilon\Omega)} = \exp\left(-\mathrm{i}\int\frac{v(\xi)2\epsilon}{\epsilon^2+\omega(\xi)^2}a^*(\xi)\mathrm{d}\xi\right)\exp\left(-\mathrm{i}\int\frac{\overline{v(\xi)}2\epsilon}{\epsilon^2+\omega(\xi)^2}a(\xi)\mathrm{d}\xi\right).$$

This converges weakly to $\mathbb{1}$.

8 Slater determinants and the Hartree-Fock method

8.1 Slater determinants

Let $\mathcal{W}$ be a Hilbert space. We consider the fermionic Fock space $\Gamma_{\rm a}(\mathcal{W})$.

Let $e_1, \dots, e_m$ be an orthonormal subset of a Hilbert space $\mathcal{W}$. Then

$$a^*(e_1)\cdots a^*(e_m)\Omega = \frac{1}{\sqrt{m!}} \sum_{\sigma\in S_m} {\rm sgn}\sigma e_{\sigma(1)}\otimes\cdots\otimes e_{\sigma(m)} \tag{8.127}$$

$$= \sqrt{m!} e_1 \otimes_{\rm a} \cdots \otimes_{\rm a} e_m = \frac{1}{\sqrt{m!}} e_1\wedge\cdots\wedge e_m \tag{8.128}$$

is a normalized vector. Such vectors are called *Slater determinants*. If $f_1, \dots, f_m$ is another basis of the subspace spanned by $e_1, \dots, e_m$, so that $e_i = \sum_j c_{ij} f_j$, then

$$a^*(e_1)\cdots a^*(e_m)\Omega = \det[c_{ij}] a^*(f_1)\cdots a^*(f_m)\Omega.$$

Let π denote the orthogonal projection on the space spanned by $e_1, \dots, e_m$. We will denote the vector (8.128) by Φ_π. (This is not quite correct, because it is fixed by π only up to a phase factor). However the the state

$$\omega_\pi(A) := \big(a^*(e_1)\cdots a^*(e_m)\Omega | A a^*(e_1)\cdots a^*(e_m)\Omega\big)$$

depends only on π.

8.2 CAR

Suppose that $e_1, e_2, \dots$ is a basis of $\mathcal{W}$. We use two conventions:

$$a_i := a(e_i), \quad a_i^* := a^*(e_i),$$

Then

$$[a_i, a_j]_+ = 0, \quad [a_i, a_j^*]_+ = \delta_{i,j}, \quad a_i\Omega = 0. \tag{8.129}$$

Alternatively, if $w = \sum w_i e_i \in \mathcal{W}$ we write

$$a(w) = \sum \overline{w}_i a_i, \quad a^*(w) = \sum w_i a_i^*,$$

We can write

$$[a(w), a(w')]_+ = 0, \quad [a(w), a_j^*(w')]_+ = (w|w'), \quad a(w)\Omega = 0. \tag{8.130}$$

The vectors $a_{i_1}^*\cdots a_{i_n}^*\Omega$, $i_1 < \cdots < i_n$ form an orthonormal basis of $\Gamma_{\rm a}(\mathcal{W})$.

8.3 Changing the vacuum

Suppose we want to treat the Slater determinant

$$\Phi := a_1^*\cdots a_n^*\Omega$$

as a new vacuum for the space $\Gamma_{\rm a}(\mathcal{W})$. One can do it as follows: we rename

$$b_i := a_i^*, \quad b_i^* := a_i, \quad i = 1, \dots, m.$$

Then we set

$$\tilde{a}_i := \begin{cases} b_i & i \le n, \\ a_j & j > n; \end{cases} \quad \tilde{a}_i^* := \begin{cases} b_i^* & i \le n, \\ a_j^* & j > n. \end{cases}.$$

Then $\tilde{a}_i, \tilde{a}_i^*, i = 1, \dots$ satisfy the usual anticommutation relations with the vacuum Φ.

Let us introduce the complex conjugation on the space $\mathbb{C}^n$ (which is embedded in $\mathcal{W}$, spanned by $e_1, \dots, e_n$:

$$\mathbb{C}^n \ni w = \sum w_n e_n \mapsto \overline{w} := \sum \overline{w}_i e_i \in \mathcal{W}.$$

Then we can set

$$\tilde{a}(w) := \sum_{i=1}^{n} b_i \overline{w}_i + \sum_{j=n+1}^{\infty} w_j a_j, \tag{8.131}$$

$$\tilde{a}^*(w) := \sum_{i=1}^{n} b_i^* \overline{w}_i + \sum_{j=n+1}^{\infty} w_j a_j^*. \tag{8.132}$$

Then $\tilde{a}(w)$, $\tilde{a}^*(w)$ satisfy the usual commutation relations with vacuum Φ

$$[\tilde{a}(w), \tilde{a}(w')]_+ = 0, \quad [\tilde{a}(w), \tilde{a}_j^*(w')]_+ = (w|w'), \quad \tilde{a}(w)\Phi = 0. \tag{8.133}$$

Thus in the new representation the 1-particle space is $\overline{\pi\mathcal{W}} \oplus (\mathbb{1} - \pi)\mathcal{W})$ and not $\mathcal{W}$. Therefore, we obtain a representation of the space $\Gamma_{\rm a}(\mathcal{W})$ as the space $\Gamma_{\rm a}(\overline{\pi\mathcal{W}} \oplus (\mathbb{1} - \pi)\mathcal{W})$.

We can implement this change (up to some signes) by a unitary transformation: Set $U := \prod_{i=1}^{m}(a_i + a_i^*)$. U satisfies

$$U a_i^* U^* = (-1)^{m+1} b_i, \quad i = 1, \dots, m; \tag{8.134}$$

$$U a_i^* U^* = (-1)^m a_i^*, \quad i = m+1, \dots \tag{8.135}$$

$$U\Omega = \Phi. \tag{8.136}$$

In fact

$$(a + a^*)a(a + a^*) = a^* a a^* = a^*(aa^* + a^* a) = a^*, \tag{8.137}$$

$$(a + a^*)a^*(a + a^*) = a a^* a = a(aa^* + a^* a) = a. \tag{8.138}$$

8.4 Free fermionic Hamiltonians

For simplicity, assume that $\mathcal{W}$ is finite dimensional. Consider $H = {\rm d}\Gamma(h)$, where h is a self-adjoint operator on $\mathcal{W}$. We can diagonalize h, so that

$$h = \sum_i \lambda_i |e_i)(e_i|.$$

It is easy to see that $\mathrm{d}\Gamma(h)$ possesses a unique ground state iff $0 \notin \mathrm{sp}h$. Indeed, let $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_m < 0 < \lambda_{m+1} \leq \ldots$. Then the ground state of $\mathrm{d}\Gamma(h)$ is given by

$$\Phi := a_1^* \cdots a_m^* \Omega,$$

so that

$$H\Phi = E\Phi, \quad E = \lambda_1 + \cdots + \lambda_m.$$

The Hamiltonian H can be rewritten as

$$H = \sum_i \lambda_i a_i^* a_i = \sum_{i \leq m} |\lambda_i| b_i^* b_i + \sum_{i>m} \lambda_i a_i^* a_i + \sum_{i \leq m} \lambda_i.$$

Note that strictly speaking this construction makes sense only for a finite dimensional $\mathbb{1}_{]-\infty,0]}(h)$. However, it is often used also if this dimension is infinite. The constant E is usually dropped—it is often in fact infinite, and we use the renormalized Hamiltonian

$$H_{\mathrm{ren}} = \sum_{i \leq m} |\lambda_i| b_i^* b_i + \sum_{i>m} \lambda_i a_i^* a_i.$$

Example 8.1 *Consider the free Fermi gas with the chemical potential μ in volume L.*

$$H = \sum_{k \in \frac{2\pi}{L}\mathbb{Z}^d} (k^2 - \mu) a_k^* a_k.$$

The ground state is called the "Fermi sea": $\prod_{k^2<\mu} a_k^* \Omega$. It has the energy

$$E = \sum_{k^2<\mu} (k^2 - \mu).$$

The renormalized Hamiltonian is

$$H_{\mathrm{ren}} = \sum_{k^2<\mu} |k^2 - \mu| b_k^* b_k + \sum_{k^2 \geq \mu} |k^2 - \mu| a_k^* a_k.$$

In infinite volume the Hamiltonian is

$$H = \int (k^2 - \mu) a_k^* a_k \mathrm{d}k.$$

E is infinite and the Slater determinant is ill defined. However, we can change the representation of CAR replacing H with

$$H_{\mathrm{ren}} = \int_{k^2<\mu} |k^2 - \mu| b_k^* b_k \mathrm{d}k + \int_{k^2 \geq \mu} |k^2 - \mu| a_k^* a_k \mathrm{d}k.$$

Example 8.2 *Consider the Dirac Hamiltonian*

$$h := \vec{\alpha}\vec{p} + \beta m + V(x).$$

It is a self-adjoint operator on $L^2(\mathbb{R}^3 \otimes \mathbb{C}^4)$ *The naive quantization of* h*, that is* $\mathrm{d}\Gamma(h)$*, acts on the space* $\Gamma_{\mathrm{a}}\big(L^2(\mathbb{R}^3 \otimes \mathbb{C}^4)\big)$*. It is however physically meaningless—it yields an operator unbounded from below. Formally, the ground state of* $\mathrm{d}\Gamma(h)$ *is the Slater determinant with all negative energy states present. This state is called the* Dirac sea.

In practice, we change the representation of CAR. Set

$$\Lambda^{\pm} := \mathbb{1}_{[0,\infty[}(\pm h).$$

The physical one particle space is

$$C\Lambda^{-} L^2(\mathbb{R}^3 \otimes \mathbb{C}^4) \oplus \Lambda^{+} L^2(\mathbb{R}^3 \otimes \mathbb{C}^4),$$

where C *is an antilinear map, usually the charge conjugation.*

8.5 CAR C^*-algebra

$\mathfrak{A}$ is a C^*-algebra if it is a Banach $*$algebra satisfying $\|A^*\| = \|A\|$ and $\|A^*A\| = \|A\|^2$. ω is a state on $\mathfrak{A}$ if it is a functional on $\mathfrak{A}$ such that $\omega(A^*A) \geq 0$ and $\omega(\mathbb{1}) = 1$. $\pi^*(\mathfrak{A}) \to B(\mathcal{H})$ is a $*$-representation if it is a $*$-homomorphism.

Every closed $*$-algebra in $B(\mathcal{H})$ is a C^*-algebra. Every functional of the form $A \mapsto \mathrm{Tr} A\rho$, where $\mathrm{Tr}\rho = 1$, $\rho \geq 0$ is a state.

The operators $a(w), a^*(w)$ with $w \in \mathcal{W}$ satisfying the CAR can be treated as abstract elements generating a $*$-algebra. After an appropriate completion it becomes a C^*-algebra, called the CAR algebra. It can be denoted $CAR(\mathcal{W})$. The representation in the Fock space $\Gamma_{\mathrm{a}}(\mathcal{W})$ is one of possible representations. I

Let π be an orthogonal projection on $\mathcal{W}$ Fix an antilinear conjugation on $\pi\mathcal{W}$, denoted by C, that is an antiunitary operator satisfying $C^2 = \mathbb{1}$. Consider the one particle Hilbert space $C\pi\mathcal{W} \oplus (\mathbb{1} - \pi)\mathcal{W}$ and the Fock space $\Gamma_{\mathrm{a}}\big(C\pi\mathcal{W} \oplus (\mathbb{1} - \pi)\mathcal{W}\big)$ Creation/annihilation operators for $Cw \in C\mathrm{Ran}\pi$ will be denoted $b^*(Cw)$ and $b(Cw)$. Then the operators

$$\rho(a^*(w)) := b(C\pi w) + a^*\big((\mathbb{1} - \pi)w\big)$$

extends to a $*$-representation of $CAR(\mathcal{W})$.

If $\mathrm{Ran}\pi$ is infinite dimensional, there is no unitary map U that intertwines the two kinds of representations of CAR. In particular, there is no vector killed by $\rho(a(w))$.

8.6 Expectation values of Slater determinants

Theorem 8.3 *Let* b *be an operator on* $\otimes^m \mathcal{W}$*. Let* π *be a projection onto a subspace of* $\mathcal{W}$*. Then*

$$\omega_\pi\big(b(a^*, a)\big) = \sum_{\sigma \in S_m} \mathrm{Tr}\, b\, \pi^{\otimes m}\, \Theta(\sigma)\mathrm{sgn}(\sigma).$$

Proof. It is enough to check this assuming that

$$b = |e_{i_1}) \cdots |e_{i_m})(e_{j_m}| \cdots (e_{j_1}|,$$

corresponding to

$$b(a^*, a) = a^*_{i_1} \cdots a^*_{i_n} a_{j_n} \cdots a_{j_1}.$$

Now

$$(a^*_1 \cdots a^*_n \Omega | a^*_{i_1} \cdots a^*_{i_m} a_{j_m} \cdots a_{j_1}\ a^*_1 \cdots a^*_n \Omega) \tag{8.139}$$

is nonzero only if $i_1, \ldots, i_m$ are distinct,

$$\{i_1, \ldots, i_m\} = \{j_1, \ldots, j_m\} \subset \{1, \ldots, n\}.$$

Then it is ± 1, where its sign is determined by the unique permutation that maps $\{i_1, \ldots, i_m\}$ onto $\{j_1, \ldots, j_m\}$. Now

$$1 = \operatorname{Tr} \pi^{\otimes m} |e_{i_1}) \cdots |e_{i_m})(e_{j_m}| \cdots (e_{j_1}| \Theta(\sigma).$$

□

In particular, we have the cases $n = 1, 2$:

$$\omega_\pi\big(\mathrm{d}\Gamma(h)\big) = \mathrm{Tr}\pi h, \tag{8.140}$$

$$\omega_\pi\big(b(a^*, a)\big) = \operatorname{Tr} b\, \pi \otimes \pi (\mathbb{1} - \tau), \tag{8.141}$$

where $\tau : \mathcal{W} \otimes \mathcal{W} \to \mathcal{W} \otimes \mathcal{W}$ is the transposition of the factors in the tensor product.

8.7 The Hartree-Fock method

Let h be a self-adjoint operator on $\mathcal{W}$ and b on $\mathcal{W} \otimes \mathcal{W}$. We assume that $\tau b \tau = b$. Consider the particle number preserving operator

$$H = \mathrm{d}\Gamma(h) + \frac{1}{2} b(a^*, a).$$

We would like to find the ground state energy of H in the n-body sector.

The Hartree-Fock functional is the expectation value of H in a Slater determinant:

$$\mathcal{E}_{\mathrm{HF}}(\pi) := \omega_\pi(H) = \mathrm{Tr} h\pi + \frac{1}{2} \operatorname{Tr} b\, \pi \otimes \pi\, (\mathbb{1} - \tau).$$

The ground state energy of H is clearly estimated from above by its Hartree-Fock energy

$$E_{\mathrm{HF}} := \inf\{\mathcal{E}_{\mathrm{HF}}(\pi)\ :\ \pi \text{ is an } n\text{-dimensional orthogonal projection}\}.$$

If a minimizer of $\mathcal{E}_{\mathrm{HF}}$ exists, we denote it by π_{HF}. We define the Hartree-Fock Hamiltonian (called also the Fock Hamiltonian) by its expectation value in a trace class matrix γ:

$$\mathrm{Tr} h_{\mathrm{HF}} \gamma := \mathrm{Tr} h\gamma + \operatorname{Tr} b\, \pi_{\mathrm{HF}} \otimes \gamma\, (\mathbb{1} - \tau).$$

Notice the absence of $\frac{1}{2}$.

Theorem 8.4 *$\pi_{\rm HF}$ is a projection onto n lowest lying levels of $h_{\rm HF}$*

Proof. Every orthogonal projection has the kernel

$$\pi(x,y) = \sum_{i=1}^{n} \overline{\phi_i(x)}\phi_i(y),$$

where $\phi_1, \ldots, \phi_n$ is an orthonormal basis of Ranπ. The Hartree-Fock functional can be written as

$$\begin{aligned}\mathcal{E}_{\rm HF}(\pi) =: \mathcal{E}(\phi_1, \ldots \phi_n) = &\sum_i (\phi_i | h\phi_i) \\ &+ \frac{1}{2}\sum_{ij} (\phi_i \otimes \phi_j | b\, \phi_i \otimes \phi_j) - \frac{1}{2}\sum_{ij} (\phi_i \otimes \phi_j | b\, \phi_j \otimes \phi_i).\end{aligned}$$

Using the method of Lagrange multipliers, $E_{\rm HF}$ is given as the infimum of

$$\mathcal{E}_{\rm HF}(\phi_1, \ldots, \phi_n) - \sum_{ij} \epsilon_{ij}\big((\phi_i|\phi_j) - \delta_{ij}\big),$$

where we may assume that the matrix ϵ_{ij} is Hermitian. Writing $\phi_i + \delta\phi_i$, $\epsilon_{ij} + \delta\epsilon_{ij}$ for the variations, we find

$$\delta\mathcal{E}_{\rm HF} = \sum_i \big(\phi_i | h_{\rm HF}\delta\phi_i\big) + \big(\delta\phi_i | h_{\rm HF}\phi_i\big) \tag{8.142}$$

$$- \sum_{ij} \epsilon_{ij}(\phi_i|\delta\phi_j) - \sum_{ij} \epsilon_{ij}(\delta\phi_i|\phi_j) \tag{8.143}$$

$$+ \sum_{ij} \delta\epsilon_{ij}\big((\phi_i|\phi_j) - \delta_{ij}\big). \tag{8.144}$$

Comparing the coefficients at $\delta\phi_i$ on the right of the scalar product and on the left of the scalar product independently, we obtain

$$h_{\rm HF}\phi_i = \sum_j \epsilon_{ij}\phi_j.$$

We can diagonalize the matrix $[\epsilon_{ij}]$ with a unitary transformation, so that $\epsilon_{ij} = \delta_{ij}\epsilon_i$, and we obtain

$$h_{\rm HF}\phi_i = \epsilon_i\phi_i.$$

Thus the minimizing sequence $\phi_1, \ldots, \phi_n$ can consist of normalized eigenvectors of $h_{\rm HF}$.

Now assume that there is an eigenvector of $h_{\rm HF}$, say ψ orthogonal to $\phi_1, \ldots \phi_n$ and with an eigenvalue β lower than one of the eigenvalues $\epsilon_1, \ldots, \epsilon_n$. For instance,

$$h_{\rm HF}\psi = \beta\psi, \quad \beta < \epsilon_1.$$

Then we can consider a variation $\phi_1 + \delta\phi_1 := \sqrt{1-t^2}\phi_1 + t\psi$. This variation is tangent to the constraints. Besides,

$$\begin{aligned}&\delta\mathcal{E}_{\rm HF}(\phi_1+\delta\phi_1,\phi_2,\dots,\phi_n)\\ =&\frac{\delta^2}{\delta\phi_1^2}\mathcal{E}_{\rm HF}\delta\phi_1\delta\phi_1+\frac{\delta^2}{\delta\overline{\phi}_1^2}\mathcal{E}_{\rm HF}\delta\overline{\phi}_1\delta\overline{\phi}_1+\frac{\delta^2}{\delta\overline{\phi}_1\delta\phi_1}\mathcal{E}_{\rm HF}\delta\overline{\phi}_1\delta\phi_1.\end{aligned}$$

The first two terms are zero because of the operator $\mathbb{1}-\tau$. The second equals

$$-t^2(\phi_1|h_{\rm HF}\phi_1)+t^2(\psi|h_{\rm HF}\psi)=t^2(-\epsilon_1+\beta),$$

hence is negative. □

Note that the Hartree-Fock energy is in general not equal to the sum of the lowest n eigenvalues of $H_{\rm HF}$.

8.8 Hartree-Fock method for atomic systems

Suppose now that $V(x)=V(-x)$ and

$$H=-\int a_x^*\Delta_x a_x\mathrm{d}x+\int a_x^*W(x)a_x\mathrm{d}x \tag{8.145}$$

$$+\frac{1}{2}\int\int a_x^*a_y^*V(x-y)a_xa_y\mathrm{d}x\mathrm{d}y. \tag{8.146}$$

Let π be an n-dimensional projection. We set

$$\rho(x):=\pi(x,x),\quad \rho_{\rm HF}(x):=\pi_{\rm HF}(x,x).$$

Then

$$\mathcal{E}_{\rm HF}(\pi)=\int\partial_x\partial_y\pi(x,y)\Big|_{x=y}\mathrm{d}x+\int W(x)\rho(x)\mathrm{d}x \tag{8.147}$$

$$+\frac{1}{2}\int\int V(x-y)\rho(x)\rho(y)\mathrm{d}x\mathrm{d}y-\frac{1}{2}\int\int V(x-y)|\pi(x,y)|^2\mathrm{d}x\mathrm{d}y,$$

$$H_{\rm HF}=-\Delta+W(x)+\int\rho_{\rm HF}(y)V(x-y)\mathrm{d}y-T_{\rm ex}, \tag{8.148}$$

where $T_{\rm ex}$ is a nonlocal operator with the kernel

$$T_{\rm ex}(x,y)=V(x-y)\pi_{\rm HF}(x,y).$$

A semiclassical argument implies that the first term in (8.147), that is the kinetic energy, can be approximated by

$$(2\pi)^{-d}\frac{d}{d+2}c_d^{-2/d}\int\rho^{\frac{d+2}{d}}(x)\mathrm{d}x, \tag{8.149}$$

where c_d is the volume of a unit ball in d dimensions. We also expect that the last term, that is the exchange energy is relatively small. This leads to the so-called Thomas-Fermi functional, which depends only on the density:

$$\begin{aligned}\mathcal{E}_{\mathrm{TF}}(\rho) :=&(2\pi)^{-d}\frac{d}{d+2}c_d^{-2/d}\int \rho^{\frac{d+2}{d}}(x)\mathrm{d}x\\ &+\int W(x)\rho(x)\mathrm{d}x+\frac{1}{2}\int\int V(x-y)\rho(x)\rho(y)\mathrm{d}x\mathrm{d}y.\end{aligned}$$

9 Squeezed states

9.1 1-mode squeezed vector

Consider $\Gamma_{\mathrm{s}}(\mathbb{C})$.

Theorem 9.1 *Let $|c|<1$. Then*

$$\Omega_c := (1-|c|^2)^{\frac{1}{4}}\mathrm{e}^{\frac{c}{2}a^{*2}}\Omega$$

is a normalized vector satisfying

$$(a-ca^*)\Omega_c = 0. \tag{9.150}$$

Proof.

$$\begin{aligned}\left(\mathrm{e}^{\frac{c}{2}a^{*2}}\Omega|\mathrm{e}^{\frac{c}{2}a^{*2}}\Omega\right) &= \sum_{n=0}^{\infty}\frac{|c|^{2n}(2n)!}{(n!)^2 2^{2n}}\\ &= \sum\frac{(-1)^n|c|^{2n}(-\frac{1}{2})(-\frac{1}{2}-1)\cdots(-\frac{1}{2}-n)}{n!} = \left(1-|c|^2\right)^{-\frac{1}{2}}.\end{aligned}$$

Using

$$\mathrm{e}^{-\frac{c}{2}a^{*2}}a\mathrm{e}^{\frac{c}{2}a^{*2}} = a-\frac{c}{2}[a^{*2},a] = a+ca^*,$$

we obtain (9.158). □

Theorem 9.2 *Set*

$$U_t := \mathrm{e}^{\frac{t}{2}(-a^{*2}+a^2)}.$$

Then

$$U_t a U_t^{-1} = a\cosh t + a^*\sinh t, \tag{9.151}$$

$$U_t a^* U_t^{-1} = a^*\cosh t + a\sinh t, \tag{9.152}$$

$$U_t = \frac{1}{\sqrt{\cosh t}}\mathrm{e}^{-\frac{\tanh t}{2}a^{*2}}\Gamma\Big(\frac{1}{\cosh t}\Big)\mathrm{e}^{\frac{\tanh t}{2}a^2}, \tag{9.153}$$

$$\Omega_{\tanh t} = U_t\Omega. \tag{9.154}$$

Proof. (9.151) and (9.152) are immediate. We next compute

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}U_t &= \frac{1}{2}(-a^{*2}+a^2)U_t \\ &= -\frac{1}{2\cosh^2 t}a^{*2}U_t + \frac{1}{2\cosh^2 t}U_t a^2 - \frac{\sinh t}{\cosh^2 t}a^* U_t a - \frac{\sinh t}{2\cosh t}U_t.\end{aligned}$$

Then we use the identity concerning the derivative of $\Gamma(\mathrm{e}^h) = \mathrm{e}^{ha^*a}$ contained in (9.155). □

Lemma 9.3

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{h(t)a^*a} = \dot{h}(t)\mathrm{e}^{h(t)}a^*\mathrm{e}^{h(t)a^*a}a. \tag{9.155}$$

Proof.

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{e}^{ha^*a} = \dot{h}\mathrm{e}^{ha^*a}a^*a \tag{9.156}$$

$$= \dot{h}\mathrm{e}^{ha^*a}a^*\mathrm{e}^{-ha^*a}\mathrm{e}^{ha^*a}a = \dot{h}\mathrm{e}^{h}a^*\mathrm{e}^{ha^*a}a. \tag{9.157}$$

□

9.2 Many-mode squeezed vector

Suppose c is a symmetric complex matrix on $\mathbb{C}^n$. One can show that then there exists an orthonormal basis such that c is diagonal where all terms on the diagonal are nonnegative. Therefore, we have the many-mode generalizations of the results of the previous subsection to $\Gamma_{\mathrm{s}}(\mathbb{C}^n)$:

Theorem 9.4 *Let c be a symmetric $n \times n$ matrix such that $\|c\| < 1$. Then*

$$\Omega_c := \det(1-|c|^2)^{\frac{1}{4}}\mathrm{e}^{\frac{1}{2}c_{ij}a_i^*a_j^*}\Omega$$

is a normalized vector satisfying

$$(a_i - c_{ij}a_j^*)\Omega_c = 0. \tag{9.158}$$

where we write $|c| := \sqrt{c^*c}$.

Theorem 9.5 *Let θ be a symmetric $n \times n$ matrix. Set*

$$U_\theta := \mathrm{e}^{\frac{1}{2}(-\theta_{ij}a_i^*a_j^* + \overline{\theta}_{ij}a_j a_i)}.$$

Then

$$U_\theta a_i U_\theta^{-1} = (\overline{\cosh|\theta|})_{ij} a_j + \Big(\theta \frac{\sinh|\theta|}{|\theta|}\Big)_{ij} a_j^*, \tag{9.159}$$

$$U_\theta a_i^* U_\theta^{-1} = (\cosh|\theta|)_{ij} a_j^* + \Big(\overline{\theta} \frac{\sinh\overline{|\theta|}}{\overline{|\theta|}}\Big)_{ij} a_j, \tag{9.160}$$

$$U_\theta = \frac{1}{\sqrt{\det\cosh|\theta|}} \mathrm{e}^{-\left(\theta \frac{\tanh|\theta|}{2|\theta|}\right)_{ij} a_i^* a_j^*} \Gamma\Big(\frac{1}{\cosh|\theta|}\Big) \mathrm{e}^{\left(\overline{\theta} \frac{\tanh\overline{|\theta|}}{2\overline{|\theta|}}\right)_{ij} a_j a_i}, \tag{9.161}$$

$$U_\theta \Omega = \Omega_{\frac{\tanh|\theta|}{|\theta|}\theta}. \tag{9.162}$$

9.3 Single-mode gauge-invariant squeezed vector

Consider $\Gamma_{\mathrm{s}}(\mathbb{C}^2)$. The creation/annihilation of first mode are denoted a^*, a, of the second b^*, b.

We assume that in our space there is a "charge operator"

$$Q := a^* a - b^* b,$$

and we are interested mostly in gauge invariant states, that is satisfying $Q = 0$.

Theorem 9.6 *Let $|c| < 1$. Then*

$$\Omega^c := (1 - |c|^2)^{\frac{1}{2}} \mathrm{e}^{c a^* b^*} \Omega$$

is a normalized vector satisfying

$$(a - c b^*)\Omega^c = 0, \tag{9.163}$$

$$(b - c a^*)\Omega^c = 0. \tag{9.164}$$

Proof.

$$\begin{aligned}\Big(\mathrm{e}^{c a^* b^*}\Omega | \mathrm{e}^{c a^* b^*}\Omega\Big) &= \sum_{n=0}^{\infty} \frac{|c|^{2n}(n!)^2}{(n!)^2} \\ &= \big(1 - |c|^2\big)^{-1}.\end{aligned}$$

Using

$$\mathrm{e}^{-c a^* b^*} a \mathrm{e}^{c a^* b^*} = a - c[a^* b^*, a] = a + c b^*,$$

we obtain (9.164). □

Remark 9.7 *Clearly,*

$$\mathrm{e}^{c a^* b^*} = \exp\Big(\frac{c}{4}(a^* + b^*)^2 - \frac{c}{4}(a^* - b^*)^2\Big).$$

Hence a single mode gauge-invariant squeezed vector can be also understood as a 2-mode squeezed state. However, it is often simple to deal with it directly.

Theorem 9.8 *Set*

$$U^t := \mathrm{e}^{t(-a^*b^*+ab)}.$$

Then

$$U^t a U^{-t} = a\cosh t + b^* \sinh t, \tag{9.165}$$

$$U^t a^* U^{-t} = a^* \cosh t + b \sinh t, \tag{9.166}$$

$$U^t b U^{-t} = b\cosh t + a^* \sinh t, \tag{9.167}$$

$$U^t b^* U^{-t} = b^* \cosh t + a \sinh t, \tag{9.168}$$

$$U^t = \frac{1}{\cosh t}\mathrm{e}^{-\tanh t a^* b^*}\Gamma\Big(\frac{1}{\cosh t}\Big)\mathrm{e}^{\tanh t ba}, \tag{9.169}$$

$$\Omega^{-\tanh t} = U^t\Omega. \tag{9.170}$$

Proof. We compute

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}U^t &= (-a^*b^* + ba)U^t \\ &= -\frac{1}{\cosh^2 t}a^*b^*U^t + \frac{1}{\cosh^2 t}U^t ba - \frac{\sinh t}{\cosh^2 t}\Big(a^*U^t a + b^*U^t b\Big) - \frac{\sinh t}{\cosh t}U^t.\end{aligned}$$

10 Bose gas and superfluidity

n identical *bosonic* particles are described by the Hilbert space

$$\mathcal{H}_n := L^2_{\mathrm{s}}\Big((\mathbb{R}^d)^n\Big) = \otimes^n_{\mathrm{s}} L^2(\mathbb{R}^d),$$

the *Schrödinger Hamiltonian*

$$H_n = -\sum_{i=1}^n \Delta_i + \lambda \sum_{1\le i<j\le n} V(x_i - x_j)$$

and the *momentum* $P_n := -\sum_{i=1}^n \mathrm{i}\partial_{x_i}$. We have $P_nH_n = H_nP_n$, which expresses the *translational invariance* of our system.
The *potential* V is a real function on $\mathbb{R}^d$ that decays at infinity and satisfies $V(x) = V(-x)$.

We enclose these particles in a box of size L with fixed density $\rho := \frac{n}{L^d}$ and n large. Instead of the more physical Dirichlet boundary conditions, to keep translational invariance we impose the *periodic boundary conditions*, replacing the original V by the *periodized potential*

$$V^L(x) \;:=\; \sum_{n\in\mathbb{Z}^d} V(x+Ln) = \frac{1}{L^d}\sum_{\mathrm{p}\in(2\pi/L)\mathbb{Z}^d} \mathrm{e}^{\mathrm{i}px}\hat{V}(\mathrm{p}),$$

well defined on the torus $[-L/2, L/2[^d$. (Note that above we used the *Poisson summation formula*).

The original Hilbert space is replaced by

$$\mathcal{H}_n^L := L^2_{\rm s}\Big(([-L/2,L/2[^d)^n\Big) = \otimes^n_{\rm s}\big(L^2([-L/2,L/2[^d)\big).$$

We have a new Hamiltonian

$$H_n^L = -\sum_{i=1}^n \Delta_i^L + \lambda \sum_{1\le i<j\le n} V^L(x_i - x_j)$$

and a new momentum $P_n^L := -\sum_{i=1}^n \mathrm{i}\partial^L_{x_i}$.

Because of the periodic boundary conditions we still have

$$P_n^L H_n^L = H_n^L P_n^L.$$

In the sequel we drop the superscript L.

We use the second quantized formalism

$$\begin{aligned}\mathcal{H} = \bigoplus_{n=0}^\infty \mathcal{H}_n &= \Gamma_{\rm s}\Big(L^2[0,L]^d\Big)\\ &\simeq \Gamma_{\rm s}\Big(l^2(\frac{2\pi}{L}\mathbb{Z}^d)\Big).\end{aligned}$$

The Hamiltonian and the momentum in second quantized notation are

$$\begin{aligned}H := \bigoplus_{n=0}^\infty H_n &= -\int a_x^*\Delta_x a_x \mathrm{d}x + \frac{\lambda}{2}\int\int \mathrm{d}x\mathrm{d}y a_x^* a_y^* V(x-y) a_y a_x\\ &= \sum_p p^2 a_p^* a_p + \frac{\lambda}{2L^d}\sum_{p,q,k}\hat V(k) a^*_{p+k}a^*_{q-k}a_q a_p,\\ P := \bigoplus_{n=0}^\infty P_n &= \int a_x^* \frac{1}{\mathrm{i}}\partial_x a_x \mathrm{d}x\\ &= \sum_p p a_p^* a_p.\end{aligned}$$

10.1 Bogoliubov's approximation in the canonical formalism

We assume that the potential is *repulsive*, more precisely,

$$\hat V \ge 0, \quad V \ge 0.$$

The Hamiltonian H commutes with N. We are interested in its low energy part for large eigenvalues n of the number of particle operator N.

We expect that for low energies most particles will be spread evenly over the whole box staying in the *zeroth mode*, so that $N \simeq N_0 := a_0^* a_0$. (The Bose statistics does not prohibit to occupy the same state). Following the arguments

of N. N. Bogoliubov from 1947, we drop all terms in the Hamiltonian involving more than two creation/annihilation operators of a nonzero mode. We obtain

$$\begin{aligned} H &\approx \frac{\lambda\hat{V}(0)}{2L^d}a_0^*a_0^*a_0a_0 + \sum_{k\neq 0}\Big(k^2 + a_0^*a_0\frac{\lambda}{L^d}\big(\hat{V}(k)+\hat{V}(0)\big)\Big)a_k^*a_k \\ &\quad + \sum_{k\neq 0}\frac{\lambda}{2L^d}\hat{V}(k)\Big(a_0^*a_0^*a_ka_{-k} + a_k^*a_{-k}^*a_0a_0\Big) \\ &= \frac{\lambda\hat{V}(0)\rho}{2}(N-1) + H_{\mathrm{Bog}} + R, \end{aligned}$$

where we set

$$\begin{aligned} \rho &= \frac{N}{L^d}, \\ H_{\mathrm{Bog}} &:= \sum_{k\neq 0}\big(k^2 + \lambda\rho\hat{V}(k)\big)a_k^*a_k \\ &\quad + \frac{1}{2}\sum_{k\neq 0}\lambda\rho\hat{V}(k)\big(a_k^*a_{-k}^* + a_ka_{-k}\big), \\ R &= -\frac{\lambda\hat{V}(0)}{2L^d}(N-N_0)(N-N_0-1) \\ &\quad + \sum_{k\neq 0}\frac{\lambda}{2L^d}\hat{V}(k)\Big((a_0^*a_0^*-N)a_ka_{-k} + a_k^*a_{-k}^*(a_0a_0-N)\Big). \end{aligned}$$

We used

$$\begin{aligned} a_0^*a_0^*a_0a_0 &= N_0(N_0-1) \\ &= N(N-1) - 2N_0(N-N_0) - (N-N_0)(N-N_0-1). \end{aligned}$$

We argue that R is small because

$$a_0^*a_0^* \approx a_0a_0 \approx N_0 \approx N.$$

A *Bogoliubov transformation*, is a linear transformation of creation/annihilation operators preserving the commutation relations. If we demand in addition that it should commute with translations, it should have the form

$$\tilde{a}_p := c_pa_p + s_pa_{-p}^*, \tag{10.171}$$

$$\tilde{a}_p^* := c_pa_p^* + s_pa_{-p}, \quad p\neq 0, \tag{10.172}$$

where

$$c_p^2 - s_p^2 = 1, \quad p\neq 0.$$

We are looking for a Bogoliubov transformation that diagonalizes the quadratic Hamiltonian H_{Bog}:

$$\begin{aligned} H_{\mathrm{Bog}} &= E_{\mathrm{Bog}} + \sum_{p\neq 0} \omega(p)\tilde{a}_p^*\tilde{a}_p, \\ P_{\mathrm{Bog}} &= \sum_{p\neq 0} p\tilde{a}_p^*\tilde{a}_p, \end{aligned}$$

This is realized by

$$\begin{aligned} c_p &:= \frac{\sqrt{|p|^2 + 2\lambda\rho\hat{V}(p)} + |p|}{2\sqrt{\omega(p)}}, \\ s_p &:= \frac{\sqrt{|p|^2 + 2\lambda\rho\hat{V}(p)} - |p|}{2\sqrt{\omega(p)}}, \\ \omega(p) &:= |p|\sqrt{|p|^2 + 2\lambda\rho\hat{V}(p)}, \\ E_{\mathrm{Bog}} &:= -\frac{1}{2}\sum_{p\neq 0}\left(|p|^2 + \lambda\rho\hat{V}(p) - |p|\sqrt{|p|^2 + 2\lambda\rho\hat{V}(p)}\right). \end{aligned}$$

$\omega(p)$ is called the *Bogoliubov dispersion relation* and E_{Bog} the *Bogoliubov energy.*

Let us show some computations:

$$\begin{aligned} & A(a_k^*a_k + a_{-k}^*a_{-k}) + B(a_k^*a_{-k}^* + a_{-k}a_k) \\ =& (Ca_k^* + Sa_{-k})(Ca_k + Sa_{-k}^*) + (Ca_k^* + Sa_{-k})(Ca_k + Sa_{-k}^*) - 2S^2, \\ \text{where}\quad & C := \frac{1}{2}(\sqrt{A+B} + \sqrt{A-B}), \\ & S := \frac{1}{2}(\sqrt{A+B} - \sqrt{A-B}). \end{aligned}$$

To obtain c_k, s_k we divide C, S by the square root of

$$C^2 - S^2 = \sqrt{A^2 - B^2}.$$

Note that $c_p = \cosh\beta_p$, $s_p = \sinh\beta_p$, where

$$\tanh(\beta_p) := \frac{|p|^2 + \lambda\rho\hat{V}(p) - |p|\sqrt{|p|^2 + 2\lambda\rho\hat{V}(p)}}{\lambda\rho\hat{V}(p)},$$

Set

$$U = \exp\Big(\sum_{p\neq 0}\frac{\beta_p}{2}\left(-a_p^*a_{-p}^* + a_pa_{-p}\right)\Big).$$

Then U is unitary and

$$\begin{aligned}
\tilde{a}_p &= U a_p U^*, \\
\tilde{a}_p^* &= U a_p^* U^*, \\
H_{\mathrm{Bog}} &= E_{\mathrm{Bog}} + U \sum_{p \neq 0} \omega(p) a_p^* a_p U^*, \\
P &= U \sum_{p \neq 0} p a_p^* a_p U^*.
\end{aligned}$$

The ground state of the Bogoliubov Hamiltonian is a squeezed state in the non-zero mode sector:

$$\frac{a_0^{*n}}{\sqrt{n!}} U \Omega.$$

The Bogoliubov dispersion relation depends on λ and ρ only through $\lambda\rho = \frac{\lambda n}{L^d}$.

The Bogoliubov Hamiltonian depends on L only through the choice of the lattice spacing $\frac{2\pi}{L}$.

We expect that the low energy part of the excitation spectra of H_n and H_{Bog} are close to one another for large n, hoping that then $n - n_0$ is small. We expect some kind of uniformity wrt L.

Note that formally we can even take the limit $L \to \infty$ obtaining

$$\begin{aligned}
H_{\mathrm{Bog}} - E_{\mathrm{Bog}} &= (2\pi)^{-d} \int \omega(p) \tilde{a}_p^* \tilde{a}_p \mathrm{d}p, \\
P &= (2\pi)^{-d} \int p \tilde{a}_p^* \tilde{a}_p \mathrm{d}p.
\end{aligned}$$

10.2 Bogoliubov's approximation in the grand-canonical approach

For a *chemical potential* $\mu > 0$, we define the *grand-canonical Hamiltonian*

$$\begin{aligned}
H_\mu := H - \mu N &= \sum_p (p^2 - \mu) a_p^* a_p \\
&\quad + \frac{\lambda}{2L^d} \sum_{p,q,k} \hat{V}(k) a_{p+k}^* a_{q-k}^* a_q a_p.
\end{aligned}$$

We will mostly set $\lambda = 1$.

If E_μ is the ground state energy of H_μ, then it is realized in the sector n satisfying

$$\partial_\mu E_\mu = -n.$$

In what follows we drop the subscript μ.

For $\alpha \in \mathbb{C}$, we define the *displacement* or *Weyl operator* of the zeroth mode: $W_\alpha := \mathrm{e}^{-\alpha a_0^* + \overline{\alpha} a_0}$. Let $\Omega_\alpha := W_\alpha \Omega$ be the corresponding *coherent vector*. Note that $P\Omega_\alpha = 0$. The *expectation of the Hamiltonian* in Ω_α is

$$(\Omega_\alpha | H \Omega_\alpha) = -\mu |\alpha|^2 + \frac{\hat{V}(0)}{2L^d} |\alpha|^4.$$

It is minimized for $\alpha = \mathrm{e}^{\mathrm{i}\tau} \frac{\sqrt{L^d \mu}}{\sqrt{\hat{V}(0)}}$, where τ is an *arbitrary phase*.

We apply the *Bogoliubov translation to the zero mode* of H by $W(\alpha)$. This means making the substitution

$$\begin{aligned} a_0 = \tilde{a}_0 + \alpha, \quad a_0^* = \tilde{a}_0^* + \overline{\alpha}, \\ a_k = \tilde{a}_k, \qquad a_k^* = \tilde{a}_k^*, \qquad k \neq 0. \end{aligned}$$

Note that

$$\tilde{a}_k = W_\alpha^* a_k W_\alpha, \quad \tilde{a}_k^* = W_\alpha^* a_k^* W_\alpha,$$

and thus the operators with and without tildes satisfy the same commutation relations. We drop the tildes.

Here is the translated Hamiltonian:

$$\begin{aligned} H \;:=\; & -L^d \frac{\mu^2}{2\hat{V}(0)} \\ & + \sum_k \Big(\frac{1}{2} k^2 + \hat{V}(k) \frac{\mu}{\hat{V}(0)} \Big) a_k^* a_k \\ & + \sum_k \hat{V}(k) \frac{\mu}{2\hat{V}(0)} \left(\mathrm{e}^{-\mathrm{i}2\tau} a_k a_{-k} + \mathrm{e}^{\mathrm{i}2\tau} a_k^* a_{-k}^* \right) \\ & + \sum_{k,k'} \frac{\hat{V}(k)\sqrt{\mu}}{\sqrt{\hat{V}(0) L^d}} (\mathrm{e}^{-\mathrm{i}\tau} a_{k+k'}^* a_k a_{k'} + \mathrm{e}^{\mathrm{i}\tau} a_k^* a_{k'}^* a_{k+k'}) \\ & + \sum_{k_1 + k_2 = k_3 + k_4} \frac{\hat{V}(k_2 - k_3)}{2L^d} a_{k_1}^* a_{k_2}^* a_{k_3} a_{k_4}. \end{aligned}$$

If we (temporarily) replace the potential $V(x)$ with $\lambda V(x)$, where λ is a (small) positive constant, the translated Hamiltonian can be rewritten as

$$H^\lambda = \lambda^{-1} H_{-1} + H_0 + \sqrt{\lambda} H_{\frac{1}{2}} + \lambda H_1.$$

Thus the 3rd and 4th terms are in some sense small, which suggests dropping them. Thus

$$H \approx -L^d \frac{\mu^2}{2\hat{V}(0)} + \mu (\mathrm{e}^{\mathrm{i}\tau} a_0^* + \mathrm{e}^{-\mathrm{i}\tau} a_0)^2 + H_{\mathrm{Bog}},$$

where

$$H_{\mathrm{Bog}} = \sum_{k\neq 0}\Big(\frac{1}{2}k^2+\hat{V}(k)\frac{\mu}{\hat{V}(0)}\Big)a_k^*a_k + \sum_{k\neq 0}\hat{V}(k)\frac{\mu}{2\hat{V}(0)}\left(\mathrm{e}^{-\mathrm{i}2\tau}a_ka_{-k}+\mathrm{e}^{\mathrm{i}2\tau}a_k^*a_{-k}^*\right)$$

Then we proceed as before obtaining the *Bogoliubov dispersion relation*

$$\omega(p)=|p|\sqrt{|p|^2+2\mu\frac{\hat{V}(p)}{\hat{V}(0)}}.$$

and the *Bogoliubov energy*

$$E_{\mathrm{Bog}}:=-\frac{1}{2}\sum_{p\neq 0}\left(|p|^2+\mu\frac{\hat{V}(p)}{\hat{V}(0)}-|p|\sqrt{|p|^2+2\mu\frac{\hat{V}(p)}{\hat{V}(0)}}\right)$$

Thus, as compared with the canonical approach, we have μ in place of $\lambda\rho$.

Note that the grand-canonical Hamiltonian H_μ is invariant wrt the $U(1)$ *symmetry* $\mathrm{e}^{\mathrm{i}\tau N}$. The parameter α has an arbitrary phase. Thus we *broke the symmetry* when translating the Hamiltonian.

The *zero mode* is not a harmonic oscillator – it has continuous spectrum and it can be interpreted as a kind of a *Goldstone mode*.

10.3 Landau's argument for superfluidity

A translation invariant system such as homogeneous Bose gas is described by a family of commuting self-adjoint operators (H,P), where $P=(P_1,\dots,P_d)$ is the momentum. If the translation invariance is on $\mathbb{R}^d$, then the momentum spectrum is $\mathbb{R}^d$. If it is in a box with periodic boundary conditions then $\mathrm{e}^{\mathrm{i}P_iL}=\mathbb{1}$, therefore the momentum spectrum is $\frac{2\pi}{L}\mathbb{Z}^d$.

We can define its *energy-momentum spectrum* $\mathrm{sp}(H,P)$.

$$\mathrm{sp}(H,P)\subset\begin{cases}\mathbb{R}\times\mathbb{R}^d, & L=\infty,\\ \mathbb{R}\times\frac{2\pi}{L}\mathbb{Z}^d, & L<\infty.\end{cases}$$

By general arguments the momentum of the ground state of a Bose gas is zero. Let E denote the *ground state energy* of H. We define the critical velocity by

$$c_{\mathrm{cr}}:=\sup\{c\ :\ H\geq E+c|P|\}.$$

Suppose that our n-body system is described with (H,P) with critical velocity c_{cr}. We add to H a perturbation u travelling at a speed w:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\Psi_t=\Big(H+\lambda\sum_{i=1}^n u(x_i-\mathrm{w}t)\Big)\Psi_t.$$

We go to the moving frame:

$$\Psi^{\mathrm{w}}_t(x_1,\dots,x_n) := \Psi_t(x_1-\mathrm{w}t,\dots,x_n-\mathrm{w}t).$$

We obtain a Schrödinger equation with a time-independent Hamiltonian

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\Psi^{\mathrm{w}}_t = \Big(H - \mathrm{w}P + \lambda\sum_{i=1}^{n} u(x_i)\Big)\Psi^{\mathrm{w}}_t.$$

Let Ψ_{gr} be the *ground state* of H. Is it *stable against a travelling perturbation*? We need to consider the *tilted Hamiltonian* $H - \mathrm{w}P$.

If $|\mathrm{w}| < c_{\mathrm{cr}}$, then $H - \mathrm{w}P \geq E$ and Ψ_{gr} is still a ground state of $H - \mathrm{w}P$. So Ψ_{gr} is stable.

If $|\mathrm{w}| > c_{\mathrm{cr}}$, then $H - \mathrm{w}P$ is unbounded from below. So Ψ_{gr} is not stable any more.

11 Fermionic Gaussian states

11.1 1-mode particle-antiparticle vector

Consider $\Gamma_{\mathrm{a}}(\mathbb{C}^2)$. The creation/annihilation of first mode are denoted a^*, a, of the second b^*, b.

We assume that in our space there is a "charge operator"

$$Q := a^*a - b^*b,$$

and we are interested mostly in states with $Q = 0$.

Theorem 11.1 *Let $c \in \mathbb{C}$. Then*

$$\Omega^c := (1+|c|^2)^{-\frac{1}{2}}\mathrm{e}^{ca^*b^*}\Omega = (1+|c|^2)^{-\frac{1}{2}}\big(\Omega + ca^*b^*\Omega\big)$$

is a normalized vector satisfying

$$(a - cb^*)\Omega^c = 0,$$
$$(b + ca^*)\Omega^c = 0.$$

Theorem 11.2 *Set*

$$U^t := \mathrm{e}^{t(-a^*b^* + ba)}.$$

Then

$$U^t a U^{-t} = a\cos t + b^*\sin t, \tag{11.173}$$
$$U^t a^* U^{-t} = a^*\cos t + b\sin t, \tag{11.174}$$
$$U^t b U^{-t} = b\cos t - a^*\sin t, \tag{11.175}$$
$$U^t b^* U^{-t} = b^*\cos t - a\sin t, \tag{11.176}$$
$$U^t = \cos t\,\mathrm{e}^{-\tan t\, a^*b^*}\Gamma\Big(\frac{1}{\cos t}\Big)\mathrm{e}^{\tan t\, ba}, \tag{11.177}$$
$$\Omega^{-\tan t} = U^t\Omega. \tag{11.178}$$

Proof. First we derive (11.173)-(11.176). Then we compute

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}U^t &= (-a^*b^* + ba)U^t \\ &= -\frac{1}{\cos^2 t}a^*b^*U^t + \frac{1}{\cos^2 t}U^t ba + \frac{\sin t}{\cos^2 t}\Big(a^*U^t a + b^*U^t b\Big) - \frac{\sin t}{\cos t}U^t.\end{aligned}$$

□

11.2 Fermionic oscillator

Let

$$H = (a^* + a)(b^* + b).$$

Theorem 11.3 *We have* $H^2 = -\mathbb{1}$, $H^* = -H$

$$\begin{aligned}\mathrm{e}^{tH} &= \cos t\mathbb{1} + \sin tH, \\ \mathrm{e}^{tH}(a^* + a)\mathrm{e}^{-tH} &= \cos 2t(a^* + a) - \sin 2t(b^* + b), \\ \mathrm{e}^{tH}(b^* + b)\mathrm{e}^{-tH} &= \cos 2t(b^* + b) + \sin 2t(a^* + a), \\ \mathrm{e}^{tH}(a^* - a)\mathrm{e}^{-tH} &= a^* - a, \\ \mathrm{e}^{tH}(b^* - b)\mathrm{e}^{-tH} &= b^* - b, \\ \Omega^{\tan t} &= \mathrm{e}^{tH}\Omega.\end{aligned}$$

In particular,

$$\begin{aligned}\mathrm{e}^{\pm\frac{\pi}{2}H} &= \pm H, \\ Ha^*H^{-1} &= -a, \qquad & HaH^{-1} &= -a^*, \\ Hb^*H^{-1} &= -b, \qquad & HbH^{-1} &= -b^*.\end{aligned}$$

12 Fermi gas and superconductivity

12.1 Fermi gas

We consider fermions with spin $\frac{1}{2}$ described by the Hilbert space

$$\mathcal{H}_n := \otimes_{\mathrm{a}}^n \left(L^2(\mathbb{R}^d, \mathbb{C}^2)\right).$$

We use the chemical potential from the beginning and we do not to assume the locality of interaction, so that the Hamiltonian is

$$H_n = -\sum_{i=1}^n \big(\Delta_i - \mu\big) + \lambda \sum_{1\le i<j\le n} v_{ij}.$$

The interaction will be given by a 2-body operator on $\otimes^2 \left(L^2(\mathbb{R}^d, \mathbb{C}^2)\right)$ given by

$$(v\Phi)_{i_1,i_2}(x_1, x_2) \;=\; \int\int v(x_1, x_2, x_3, x_4)\Phi_{i_1,i_2}(x_3, x_4)\mathrm{d}x_3\mathrm{d}x_4.$$

We will assume that v is invariant wrt the exchange of particles, Hermitian, real and translation invariant:

$$\begin{aligned} v(x_1,x_2,x_3,x_4) &= v(x_2,x_1,x_4,x_3) \\ &= \overline{v(x_1,x_2,x_3,x_4)} \\ &= \overline{v(x_4,x_3,x_2,x_1)} \\ &= v(x_1+y,x_2+y,x_3+y,x_4+y). \end{aligned}$$

By the invariance wrt the exchange of particles v preserves $\otimes_{\mathrm{a}}^2 \big(L^2(\mathbb{R}^d,\mathbb{C}^2)\big)$. By translation invariance, v can be written as

$$\begin{aligned} v(x_1,x_2,x_3,x_4) = (2\pi)^{-4d} \int \mathrm{e}^{\mathrm{i}k_1x_1+\mathrm{i}k_2x_2-\mathrm{i}k_3x_3-\mathrm{i}k_4x_4} q(k_1,k_2,k_3,k_4) \\ \times \delta(k_1+k_2-k_3-k_4)\mathrm{d}k_1\mathrm{d}k_2\mathrm{d}k_3\mathrm{d}k_4, \end{aligned}$$

where q is a function defined on the subspace $k_1+k_2=k_3+k_4$. An example of such interaction is a local 2-body potential $V(x)$ such that $V(x)=V(-x)$, which corresponds to

$$\begin{aligned} v(x_1,x_2,x_3,x_4) &= V(x_1-x_2)\delta(x_1-x_4)\delta(x_2-x_3), \\ q(k_1,k_2,k_3,k_4) &= \int \mathrm{d}\mathrm{p}\hat{V}(\mathrm{p})\delta(k_1-k_4-\mathrm{p})\delta(k_2-k_3+\mathrm{p}). \end{aligned}$$

Similarly, as before, we periodize the interaction

$$\begin{aligned} & v^L(x_1,x_2,x_3,x_4) \\ = & \sum_{\mathrm{n}_1,\mathrm{n}_2,\mathrm{n}_3\in\mathbb{Z}^d} v(x_1+\mathrm{n}_1L,x_2+\mathrm{n}_2L,x_3+\mathrm{n}_3L,x_4) \\ = & \frac{1}{L^{3d}} \sum_{k_1+k_2=k_3+k_4} \mathrm{e}^{\mathrm{i}k_1\cdot x_1+\mathrm{i}k_2x_2-\mathrm{i}k_3x_3-\mathrm{i}k_4x_4} q(k_1,k_2,k_3,k_4), \end{aligned}$$

where $k_i \in \frac{2\pi}{L}\mathbb{Z}^d$. The Hamiltonian

$$H^{L,n} = \sum_{1\le i\le n} \big(-\Delta_i^L - \mu\big) + \sum_{1\le i<j\le n} v_{ij}^L$$

acts on $\mathcal{H}^{n,L} := \otimes_{\mathrm{a}}^n \big(L^2([-L/2,L/2]^d,\mathbb{C}^2)\big)$. We drop the superscript L.

We will denote the spins by $i=\uparrow,\downarrow$. It is convenient to put all the n-particle spaces into a single Fock space

$$\overset{\infty}{\underset{n=0}{\oplus}} \mathcal{H}^n = \Gamma_{\mathrm{a}}\big(L^2([L/2,L/2]^d,\mathbb{C}^2)\big)$$

and rewrite the Hamiltonian and momentum in the language of 2nd quantization:

$$H := \bigoplus_{n=0}^{\infty} H^n = \sum_i \int a^*_{x,i}(\Delta_x - \mu) a_{x,i_2} \mathrm{d}x$$
$$+ \frac{1}{2} \sum_{i_1,i_2} \int\int a^*_{x_1,i_1} a^*_{x_2,i_2} v(x_1,x_2,x_3,x_4) a_{x_3,i_2} a_{x_4,i_1} \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}x_3 \mathrm{d}x_4,$$
$$P := \bigoplus_{n=0}^{\infty} P^n = -\sum_i \mathrm{i} \int a^*_{x,i} \nabla_x a_{x,i} \mathrm{d}x.$$

In the momentum representation,

$$\begin{aligned} H &= \sum_i \sum_k (k^2 - \mu) a^*_{k,i} a_{k,i} \\ &+ \frac{1}{2L^d} \sum_{i_1,i_2} \sum_{k_1+k_2=k_3+k_4} q(k_1,k_2,k_3,k_4) a^*_{k_1,i_1} a^*_{k_2,i_2} a_{k_3,i_2} a_{k_4,i_1}, \\ P &= \sum_i \sum_k k a^*_{k,i} a_{k,i}. \end{aligned}$$

We also have the generators of the spin $su(2)$.

$$S_x = \frac{1}{2} \sum_k (a^*_{k\uparrow} a_{k\downarrow} + a^*_{k\downarrow} a_{k\uparrow}), \tag{12.179}$$
$$S_y = \frac{\mathrm{i}}{2} \sum_k (a^*_{k\uparrow} a_{k\downarrow} - a^*_{k\downarrow} a_{k\uparrow}), \tag{12.180}$$
$$S_z = \frac{1}{2} \sum_k (a^*_{k\uparrow} a_{k\uparrow} - a^*_{k\downarrow} a_{k\downarrow}). \tag{12.181}$$

The Hamiltonian is invariant with respect to the spin $su(2)$.

13 Hartree-Fock-Bogoliubov approximation with BCS ansatz

We try to compute the excitation spectrum of the Fermi gas by approximate methods. We look for a minimum of the energy among Gaussian states. We assume that a minimizer is invariant wrt translations and the spin $su(2)$. We use the Hartree-Fock-Bogoliubov approximation with the Bardeen-Cooper-Schrieffer ansatz.

For a sequence $\frac{2\pi}{L}\mathbb{Z}^d \ni k \mapsto \theta_k$ such that $\theta_k = \theta_{-k}$, set

$$U_\theta := \prod_k \mathrm{e}^{\frac{1}{2}\theta_k(-a^*_{k\uparrow}a^*_{-k\downarrow} + a_{-k\downarrow}a_{k\uparrow} - a^*_{-k\uparrow}a^*_{k\downarrow} + a_{k\downarrow}a_{-k\uparrow})}.$$

(Note the double counting for $k \neq 0$). We are looking for a minimizer of the form $U_\theta \Omega$.

Note that U_θ commutes with P and the spin $su(2)$. Therefore, $U_\theta\Omega$ is translation and $su(2)$ invariant.

We want to compute

$$(U_\theta\Omega|HU_\theta\Omega) = (\Omega|U_\theta^* H U_\theta\Omega).$$

To do this we can use the fact that U_θ implements Bogoliubov rotations:

$$\begin{aligned}
U_\theta^* a_{k\uparrow}^* U_\theta &= \cos\theta_k a_{k\uparrow}^* + \sin\theta_k a_{-k\downarrow},\\
U_\theta^* a_{k\uparrow} U_\theta &= \cos\theta_k a_{k\uparrow} + \sin\theta_k a_{-k\downarrow}^*,\\
U_\theta^* a_{k\downarrow}^* U_\theta &= \cos\theta_k a_{k\downarrow}^* - \sin\theta_k a_{-k\uparrow},\\
U_\theta^* a_{k\downarrow} U_\theta &= \cos\theta_k a_{k\downarrow} - \sin\theta_k a_{-k\uparrow}^*,
\end{aligned}$$

Afteer inserting this into $U_\theta^* H U_\theta$ be can Wick order the obtained expression.

In practice, this is usually presented differently. One makes the substitution

$$\begin{aligned}
a_{k\uparrow} &= \cos\theta_k b_{k\uparrow}^* + \sin\theta_k b_{-k\downarrow},\\
a_{k\uparrow} &= \cos\theta_k b_{k\uparrow} + \sin\theta_k b_{-k\downarrow}^*,\\
a_{k\downarrow}^* &= \cos\theta_k b_{k\downarrow}^* - \sin\theta_k b_{-k\uparrow},\\
a_{k\downarrow} &= \cos\theta_k b_{k\downarrow} - \sin\theta_k b_{-k\uparrow}^*,
\end{aligned}$$

in the Hamiltonian. Note that

$$\begin{aligned}
U_\theta a_{k\uparrow}^* U_\theta^* &= b_{k\uparrow}^*,\\
U_\theta a_{k\uparrow} U_\theta^* &= b_{k\uparrow},\\
U_\theta a_{k\downarrow}^* U_\theta^* &= b_{k\downarrow}^*,\\
U_\theta a_{k\downarrow} U_\theta^* &= b_{k\downarrow}.
\end{aligned}$$

Then one Wick orders wrt the operators B^*, b. Our Hamiltonian becomes

$$\begin{aligned}
H = B &+ \sum_k D(k)\big(b_{k\uparrow}^* b_{k\uparrow} + b_{k\downarrow}^* b_{k\downarrow}\big)\\
&+ \frac{1}{2}\sum_k O(k)\big(b_{k\uparrow}^* b_{-k\downarrow}^* + b_{-k\uparrow}^* b_{k\downarrow}^*\big) + \frac{1}{2}\sum_k \overline{O}(k)\big(b_{-k\downarrow} b_{k\uparrow} + b_{k\downarrow} b_{-k\uparrow}\big)\\
&+ \text{terms higher order in } b\text{'s}.
\end{aligned}$$

Note that

$$(\Omega_\theta|H\Omega_\theta) = B.$$

By the Beliaev Theorem, minimizing B is equivalent to $O(k) = 0$.

If we choose the Bogoliubov transformation according to the minimization procedure, the Hamiltonian equals

$$H = B + \sum_k D(k)\big(b_{k\uparrow}^* b_{k\uparrow} + b_{k\downarrow}^* b_{k\downarrow}\big) + \text{terms higher order in } b\text{'s}$$

with

$$\begin{aligned} B &= \sum_k (k^2-\mu)(1-\cos 2\theta_k) \\ &\quad + \frac{1}{4L^d}\sum_{k,k'} \alpha(k,k')\sin 2\theta_k \sin 2\theta_{k'} \\ &\quad + \frac{1}{4L^d}\sum_{k,k'} \beta(k,k')(1-\cos 2\theta_k)(1-\cos 2\theta_{k'}). \end{aligned}$$

Here,

$$\begin{aligned} \alpha(k,k') &:= \frac{1}{2}\big(q(k,-k,-k',k') + q(-k,k,-k',k')\big), \\ \beta(k,k') &= 2q(k,k',k',k) - q(k',k,k',k). \end{aligned}$$

In particular, in the case of local potentials we have

$$\begin{aligned} \alpha(k,k') &:= \frac{1}{2}\big(\hat{V}(k-k') + \hat{V}(k+k')\big), \\ \beta(k,k') &= 2\hat{V}(0) - \hat{V}(k-k'). \end{aligned}$$

The condition $\partial_{\theta_k} B = 0$, or equivalently $O(k) = 0$, has many solutions. We can have

$$\sin 2\theta_k = 0, \qquad \cos 2\theta_k = \pm 1,$$

They correspond to *Slater determinants* and have a fixed number of particles. The solution of this kind minimizing B, is called the *normal* or *Hartree-Fock solution*.

Under some conditions the global minimum of B is reached by a non-normal configuration satisfying

$$\sin 2\theta_k = -\frac{\delta(k)}{\sqrt{\delta^2(k)+\xi^2(k)}}, \qquad \cos 2\theta_k = \frac{xi(k)}{\sqrt{\delta^2(k)+\xi^2(k)}},$$

where

$$\begin{aligned} \delta(k) &= \frac{1}{2L^d}\sum_{k'} \alpha(k,k')\sin 2\theta_{k'}, \\ \xi(k) &= k^2 - \mu + \frac{1}{2L^d}\sum_{k'} \beta(k,k')(1-\cos 2\theta_{k'}), \end{aligned}$$

and at least some of $\sin 2\theta_k$ are different from 0. It is sometimes called a *superconducting solution*.

For a superconducting solution we get

$$D(k) = \sqrt{\xi^2(k) + \delta^2(k)}.$$

Thus we obtain a positive dispersion relation. One can expect that it is strictly positive, since otherwise the two functions δ and ξ would have a coinciding zero, which seems unlikely. Thus we expect that the dispersion relation $D(k)$ has a *positive energy gap*.

Conditions guaranteeing that a superconducting solution minimizes the energy should involve some kind of negative definiteness of the quadratic form α – this is what we vaguely indicated by saying that the interaction is *attractive*. Indeed, multiply the definition of $\delta(k)$ with $\sin 2\theta_k$ and sum it up over k. We then obtain

$$\begin{aligned} & \sum_k \sin^2 2\theta_k \sqrt{\delta^2(k) + \xi^2(k)} \\ = \quad & -\frac{1}{2L^d} \sum_{k,k'} \sin 2\theta_k \alpha(k,k') \sin 2\theta_{k'}. \end{aligned}$$

The left hand side is positive. This means that the quadratic form given by the kernel $\alpha(k,k')$ has to be negative at least at the vector given by $\sin 2\theta_k$.