Second Quantization from a Mathematical Point of View

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SFB-Tr 12 - Bad Honnef 2009

Canonical Anti-Commutation Relations

CAR

Anti-commutator

$$\{a, a^\dagger\} = aa^\dagger + a^\dagger a = \mathbb{1}$$

with two types of operators.
Canonical anti-commutation relations (CAR) $\rightsquigarrow$ fermions

CCR

Commutator

$$[a, a^\dagger] = aa^\dagger - a^\dagger a = \mathbb{1}$$

with two types of operators.
Canonical commutation relations (CCR) $\rightsquigarrow$ bosons

Setting

- Need more than one a, $a^\dagger$
  - Index space: L complex vector space with scalar product, i.e. a Hilbert space
- Need a space where the operators act
  - Representation space: $\mathcal{F}$ complex Hilbert space.
- Conclusion: For each $f \in L$ there are linear operators $a(f)$, $a^\dagger(f) : \mathcal{F} \to \mathcal{F}$ with

$$a(\alpha f + \beta g) = \alpha a(f) + \beta a(g)$$

and

$$a^\dagger(\alpha f + \beta g) = \alpha a^\dagger(f) + \beta a^\dagger(g)$$

$\rightsquigarrow$ operator-valued functionals

Fock representation

1. Anti-commutators ($f \mapsto \bar{f}$ conjugation on L)

$$\{a(f), a(g)\} = 0 = \{a^\dagger(f), a^\dagger(g)\}$$
$$\{a(f), a^\dagger(g)\} = (\bar{f}, g)\mathbb{1}$$

2. Unitarity

$$a(f)^* = a^\dagger(\bar{f})$$

3. Vacuum vector
   3.1 Annihilation operators: $\exists \Omega \in \mathcal{F}$, $\|\Omega\| = 1$ with

   $$a(f)\Omega = 0 \text{ for all } f \in L$$

   3.2 Creation operators: $\mathcal{F}$ smallest Hilbert space containing all

   $$a^\dagger(f_n) \cdots a^\dagger(f_1)\Omega, \; n \in \mathbb{N}_0$$

$\rightsquigarrow$ Fock representation of the CAR. $\mathcal{F}$ Fock space

Alternative frameworks

Index Version

- $\{e_j\}$ complete orthonormal system in L. Define

$$a_j := a(e_j), \; a_j^\dagger := a^\dagger(\bar{e}_j)$$

- Unitarity $a_j^* = a_j^\dagger$
- CAR

$$\{a_j, a_k\} = 0 = \{a_j^\dagger, a_k^\dagger\}$$
$$\{a_j, a_k^\dagger\} = \delta_{jk}\mathbb{1}$$

  with δ_{jk} Kronecker delta
- Equivalent to present approach (for separable L)

Alternative frameworks

Operator-valued functions

- Formally

$$a(f) = \int f(x)a(x)\,dx, \;\; a^\dagger(f) = \int f(x)a^\dagger(x)\,dx$$

$a(x)$, $a^\dagger(x)$ operator-valued functions

- CAR

$$\{a(x), a(y)\} = 0 = \{a^\dagger(x), a^\dagger(y)\}$$
$$\{a(x), a^\dagger(y)\} = \delta(x-y)\mathbb{1}$$

with $\delta(x)$ Dirac delta (singular quantity)

- Problem: $a^\dagger(x)$ is NOT a well-defined operator
- Smear out $a(x)$, $a^\dagger(x)$ with a test function

Algebraic structure of the Fock space $\mathcal{F}$

- n-particle spaces

$$\mathcal{F}^{(n)} := \text{linear combinations}\{a^\dagger(f_n)\cdots a^\dagger(f_1)\Omega\},\ \ n \in \mathbb{N}_0.$$

- Decomposition

$$\mathcal{F} = \bigoplus_{n=0}^{\infty} \mathcal{F}^{(n)}.$$

- Due to the CAR

$$(f_1,\dots,f_n) \mapsto a^\dagger(f_n)\cdots a^\dagger(f_1)\Omega$$

  is alternating and multilinear. Hence,

$$\mathcal{F}^{(n)} \simeq \underbrace{L\wedge\ldots\wedge L}_{n-\text{times}} \text{ anti-symmetric tensor product}$$

- $\mathcal{F}$ is the anti-symmetric tensor algebra over L.

Hilbert space structure of the Fock space $\mathcal{F}$

- n-particle spaces are orthogonal

$$\mathcal{F}^{(m)} \perp \mathcal{F}^{(n)}, \;\; m \neq n$$

- Scalar products $\rightsquigarrow$ Slater determinants

$$(a^\dagger(f_n)\cdots a^\dagger(f_1)\Omega, a^\dagger(g_n), \cdots a^\dagger(g_1)\Omega) = \begin{vmatrix} (f_1, g_1) & \dots & (f_1, g_n) \\ \vdots & & \vdots \\ (f_n, g_1) & \dots & (f_n, g_n) \end{vmatrix}$$

- Uniqueness $\mathcal{F}$ completely determined by L
- $a(f)$ and $a^\dagger(f)$ are bounded and depend continuously on f

$$\|a(f)\| \leq \|f\|, \;\; \|a^\dagger(f)\| \leq \|f\|$$

Note: Boson operators are unbounded $\rightsquigarrow$ Wieland-Wintner theorem

Operators on the Fock space $\mathcal{F}$

Orthonormal system $\{e_j\}$ in L. $A, B, C \in B(L)$.

$$\Delta(A) := \sum_j a(Ae_j)a(\bar{e}_j), \;\; \Delta^+(C) := \sum_j a^\dagger(Ce_j)a^\dagger(\bar{e}_j)$$

$$d\Gamma(B) := \sum_j a^\dagger(Be_j)a(\bar{e}_j)$$

Quadratic operators: Well-defined? Analytical properties?

Particle number operator

$$N := d\Gamma(\mathbb{1}) = \sum_j a^\dagger(e_j)a(\bar{e}_j)$$

Indicates the particle space

$$Na^\dagger(f_n)\cdots a^\dagger(f_1)\Omega = na^\dagger(f_n)\cdots a^\dagger(f_1)\Omega$$

Well-definedness

Important tool: N^τ-estimates. The literature has

$$\|\Delta(A)\Phi\| \leq \|A\|_2\|N\Phi\|, \ \|A\|_2 := (\operatorname{tr} A^*A)^{\frac{1}{2}} \ \text{(Hilbert-Schmidt norm)}$$

We can do better

$$\|\Delta(A)\Phi\| \leq \|A\|_2\|(N+\mathbb{1})^{\frac{1}{2}}\Phi\|$$

Allows to define $\Delta(A)$ on $D(N^{\frac{1}{2}})$ instead of $D(N)$.
Some properties

- $\Delta(A)$ and $\Delta^+(C)$ need only $A^T = -A$, $C^T = -C$ (A^T transpose).
- $\Delta(A)$ and $\Delta^+(C)$ are well-defined if and only if $A, C \in B_2(L)$.
- $d\Gamma(B)$ is well-defined if and only if $B \in B(L)$. No anti-symmetry!

Boundedness

- A tool from spectral theory. Singular value decomposition

$$Cf = \sum_j \lambda_j (e_j, f) f_j$$

- When C trace class then $\Delta^+(C)$ bounded (false for bosons!)

$$\begin{aligned} \|\Delta^+(C)\| &= \|\sum_j a^\dagger(Ce_j)a(\bar{e}_j)\| \\ &\leq \sum_j \|a^\dagger(Ce_j)a(\bar{e}_j)\| \\ &\leq \sum_j |\lambda_j| \\ &< \infty \end{aligned}$$

- When $\Delta^+(C)$ bounded then? Needs more machinery!

Exponential functions

We study

$$e^{t\Delta^+(C)}, \; t \in \mathbb{C}, \; C \in B_2(L).$$

Bosons: Squeezing operators. In particular BCS states or fermionic Gaussians

$$e^{t\Delta^+(C)}\Omega$$

Well-defined because of $N^{\frac{1}{2}}$-estimate

$$\begin{aligned} \|e^{t\Delta^+(C)}\Omega\|^2 &= \sum_{n=0}^{\infty} \frac{t^{2n}}{(n!)^2} \|\Delta^+(C)^n\Omega\|^2 \\ &\leq \sum_{n=0}^{\infty} \frac{n!}{(n!)^2} 2^n t^{2n} \|C\|_2^{2n} \\ &< \infty \end{aligned}$$

for all $t \in \mathbb{C}$ and $C \in B_2(L)$. No restriction $\|C\|_2 < 1$ needed.

Commutators

- Functor of second quantization

$$[d\Gamma(B_1), d\Gamma(B_2)] = d\Gamma([B_1, B_2])$$

- Scalar terms

$$[\Delta(A), \Delta^+(C)] = -4d\Gamma(CA) + 2\,\mathrm{tr}\,AC\,\mathbb{1}.$$

- General commutator

$$\Xi(A, B, C) := \Delta(A) + d\Gamma(B) + \Delta^+(C) \leftrightarrow \begin{pmatrix} -B^T & 2A \\ 2C & B \end{pmatrix}$$

$$[\Xi(A_1, B_1, C_1), \Xi(A_2, B_2, C_2)] = \Xi([(1), (2)]) + 2\,\mathrm{tr}(A_1C_2 - A_2C_1)\mathbb{1}$$

- Helps to systemize computations

Lie algebras

- Block matrices

$$\mathfrak{so}(L) = \left\{ \begin{pmatrix} -B^T & A \\ C & B \end{pmatrix}, \; A^T = -A, \; C^T = -C \right\}$$

$\rightsquigarrow$ orthogonal Lie algebra

- $\Xi(A, B, C)$ give central extension of $\mathfrak{so}_{res}(L)$
  $\rightsquigarrow$ metagonal Lie algebra
- $\mathrm{tr}(A_1 C_2 - A_2 C_1)$ is called
  - Schwinger term (in physics)
  - Kac-Peterson cocycle (in mathematics)
- Bosons
  - Block matrices: symplectic Lie algebra
  - Central extension: metaplectic Lie algebra

A scalar factor

- Vacuum expectation value

$$\omega(t) := (\Omega, e^{t\Delta(A)} e^{t\Delta^+(C)}\Omega)$$

- Differential equation

$$\omega'(t) = \gamma(t)\omega(t)$$

- γ contains the trace from the commutator.
- Vacuum expectation value $\rightsquigarrow$ Fredholm determinant

$$(\Omega, e^{t\Delta(A)} e^{t\Delta^+(C)}\Omega)^2 = \det(\mathbb{1} + 4t^2 AC)$$

- $n \times n$-Slater determinant

$$\omega_n(t) := (a^\dagger(g_n)\cdots a^\dagger(g_1)\Omega, e^{t\Delta(A)} e^{\Delta^+(C)} a^\dagger(h_n)\cdots a^\dagger(h_1)\Omega)$$

- With appropriate functions $g_j(t)$, $h_j(t)$

$$\omega_n(t)^2 = \omega_n(0)^2 \det(\mathbb{1} + 4t^2 AC)$$

Application

- Assume $\Delta^+(C)$ bounded
- Estimate

$$d(t) := \det(\mathbb{1} + 4t^2 C^* C) = (\Omega, e^{t\Delta(C^*)} e^{t\Delta^+(C)} \Omega)^2 \leq e^{4|t|\delta}.$$

- d is an entire function of exponential order 1
- Zeros $\mu_j \neq 0$ of d

$$\sum_{j=1}^{\infty} \frac{1}{|\mu_j|^\alpha} < \infty, \ \forall \alpha > 1$$

- λ_j singular values. C is 'nearly' trace class

$$\sum_{j=1}^{\infty} \lambda_j^\alpha < \infty, \ \forall \alpha > 1, \ \mu_j = \pm \frac{i}{2\lambda_j}$$

- Open question: Does $\Delta^+(C)$ bounded imply C trace class?

Bogoliubov transforms

- Produce new representations. Simplest idea

$$b(f) = a(Sf) + a^\dagger(Tf)$$
$$b^\dagger(f) = a(\bar{T}f) + a^\dagger(\bar{S}f) \quad \leftarrow \text{unitarity!}$$

with $S, T \in B(L)$, $\bar{S}$, $\bar{T}$ conjugated operators.

- CAR satisfied if and only if

$$S^T T + T^T S = 0 \qquad \{b(f), b(g)\} = 0$$
$$S^* S + T^* T = \mathbb{1} \qquad \{b(f), b^\dagger(g)\} = (\bar{f}, g)\mathbb{1}$$

With block matrices

$$\begin{pmatrix} S & \bar{T} \\ T & \bar{S} \end{pmatrix}^* \begin{pmatrix} S & \bar{T} \\ T & \bar{S} \end{pmatrix} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix}$$

- On the Lie algebra $\rightsquigarrow$ inner automorphisms of $\mathfrak{so}(L)$

Quasi-free representation

- Start with a Fock representation
- Apply a Bogoliubov transform
- New representation is called quasi-free representation
- Question When is a quasi-free representation unitary equivalent to the underlying Fock representation?

$$b(f) = Ua(f)U^*, \; b^\dagger(f) = Ua^\dagger(f)U^*$$

with $U : \mathcal{F} \to \mathcal{F}$ unitary.

Theorem (Shale-Stinespring)

A Bogoliubov transform is a unitary transform if and only if T is a Hilbert-Schmidt operator, i.e. $\operatorname{tr} T^* T < \infty$.

Proof: Look for a new vacuum!

The new vacuum

- Important quantity

$$\ker(S) = \{f \in L | Sf = 0\}$$

Bosons S is injective!

- When T Hilbert-Schmidt then $\dim \ker(S) < \infty$
- Explicit form

$$\tilde{\Omega} = a^\dagger(Tf_d) \cdots a^\dagger(Tf_1) e^{-\frac{1}{2}\Delta^+(TS^\sim)} \Omega$$

where

  - $f_1, \dots, f_d$ is a basis for $ker(S)$
  - $S^\sim$ is a pseudo-inverse of S

- Estimate

$$\|\tilde{\Omega}\|^4 \leq c_d \det(\mathbb{1} + (TS^\sim)^* TS^\sim)$$

Bosonization T NOT Hilbert-Schmidt then possibly $\dim \ker(S) = \infty$.

Example

- L with orthonormal system e_j, $j \in \mathbb{Z}$
- Index version: $a_j := a(e_j)$, $a_j^\dagger := a^\dagger(\bar{e}_j)$
- Bogoliubov transform: S, T projection operators

$$S : L \to \{e_j, j > 0\},\ \ T : L \to \{e_j, j \leq 0\}$$

- Explicitely $\rightsquigarrow$ interchange some creation and annihilation operators

$$b_j = a_j,\ \ b_j^\dagger = a_j^\dagger,\ \ j > 0$$
$$b_j = a_j^\dagger,\ \ b_j^\dagger = a_j,\ \ j \leq 0$$

- Vacuum

$$b_j\Omega = 0,\ \ j > 0,\ \ b_j^\dagger\Omega = 0,\ \ j \leq 0$$

$\rightsquigarrow$ Dirac sea, particle/anti-particle creation operators

- No unitary transform

Bosons from Fermions

Construct a representation of the
Canonical Commutation relations (CCR)

$$[c(f), c(g)] = 0 = [c^\dagger(f), c^\dagger(g)]$$
$$[c(f), c^\dagger(g)] = (\bar{f}, g)\mathbb{1}$$

in the fermionic Fock space!

Two points of view

- Bosonization
  - First step: Construct bosonic operators in the fermionic Fock space!
  - Second step: Diagonalize some concrete Hamilton operator!
- Boson-fermion correspondence
  - First half: Get bosons from fermions!
  - Second half: Get fermions from bosons!

Usual approach

- Take the special quasi-free representation

$$b_j = a_j,\ b_j^\dagger = a_j^\dagger,\ j > 0$$
$$b_j = a_j^\dagger,\ b_j^\dagger = a_j,\ j \leq 0.$$

  Recall: NO Fock representation!

- Define fermionic currents

$$c_j := \sum_{k=-\infty}^{\infty} b_{k-j}^\dagger b_k,\ c_j^\dagger := \sum_{k=-\infty}^{\infty} b_{k+j}^\dagger b_j$$

  These give (essentially) a representation of CCR

$$[c_j, c_k^\dagger] \sim \delta_{jk} \mathbb{1}$$

General approach

- Recall

$$[\Xi(A_1, B_1, C_1), \Xi(A_2, B_2, C_2)] = \Xi([(1), (2)]) + 2\,\mathrm{tr}(A_1 C_2 - A_2 C_1)\mathbb{1}$$

- When
$$\left[\begin{pmatrix} -B_1^T & 2C_1 \\ 2A_1 & B_1 \end{pmatrix}, \begin{pmatrix} -B_2^T & 2C_2 \\ 2A_2 & B_2 \end{pmatrix}\right] = 0$$
then
$$[\Xi(A_1, B_1, C_1), \Xi(A_2, B_2, C_2)] = 2\,\mathrm{tr}(A_1 C_2 - A_2 C_1)\mathbb{1}$$
$\rightsquigarrow$ looks like CCR!
- Find commuting block matrices!
- On the Lie algebra $\mathfrak{so}(L)$: Find (all) abelian subalgebras!

Commuting block matrices

- Take commuting operators $\{B\}$.
- Define commuting block matrices

$$\begin{pmatrix} -B^T & 0 \\ 0 & B \end{pmatrix}$$

- Apply a fixed Bogoliubov transform

$$\begin{pmatrix} S & \bar{T} \\ T & \bar{S} \end{pmatrix} \begin{pmatrix} -B^T & 0 \\ 0 & B \end{pmatrix} \begin{pmatrix} S & \bar{T} \\ T & \bar{S} \end{pmatrix}^*$$

  Still commuting operators.
- Formally $\rightsquigarrow$

$$\begin{aligned} d\hat{\Gamma}(B) &= \sum_j b^\dagger(Be_j) b(\bar{e}_j) \\ &= \Delta(\tilde{A}) + d\Gamma(\tilde{B}) + \Delta^+(\tilde{C}) + const\,\mathbb{1} \\ &= \Xi(\tilde{A}, \tilde{B}, \tilde{C}) + const\,\mathbb{1} \end{aligned}$$

Commuting operators

- Quasi-free representation L with orthonormal system e_j, $j \in \mathbb{Z}$

$$b_j = a_j,\ \ b_j^\dagger = a_j^\dagger,\ \ j > 0$$
$$b_j = a_j^\dagger,\ \ b_j^\dagger = a_j,\ \ j \leq 0$$

- Choose $L = L^2[-\pi, \pi]$.
- Orthonormal system $e_j(x) = \frac{1}{\sqrt{2\pi}} e^{ijx}$.
- B multiplication operator

$$(Bf)(x) = b(x)f(x)$$

- When $b(x) = e_j(x)$

$$(Be_k)(x) = e_j(x)e_k(x) = e_{j+k}(x)$$

$\rightsquigarrow$ fermionic current c_j, $c_j^\dagger$

Bosonic vacua

- Bogoliubov transform

$$b(f) = a(Sf) + a^\dagger(Tf),\ \ b^\dagger(f) = a(\bar{T}f) + a^\dagger(\bar{S}f)$$

- Formally

$$d\hat{\Gamma}(B) = \sum_j b^\dagger(Be_j)b(\bar{e}_j)$$

- Bosonic vacua

$$d\hat{\Gamma}(B)\Omega_b = 0$$

- New fermionic vacuum

$$\tilde{\Omega} = a^\dagger(Tf_d)\cdots a^\dagger(Tf_1)e^{-\frac{1}{2}\Delta^+(TS^\sim)}\Omega$$

- Partial vacua $0 \leq d' \leq d$

$$\Omega_{d'} := a^\dagger(Tf_{d'})\cdots a^\dagger(Tf_1)e^{-\frac{1}{2}\Delta^+(TS^\sim)}\Omega$$

Bosonic annihilation operators

- Formal operators

$$d\hat{\Gamma}(B) = \sum_j b^\dagger(Be_j)b(\bar{e}_j)$$

- Vacuum property

$$\begin{aligned} d\hat{\Gamma}(B)\Omega_{d'} &= \sum_j b^\dagger(Be_j)b(\bar{e}_j)a^\dagger(Tf'_d)\cdots a^\dagger(Tf_1)e^{-\frac{1}{2}\Delta^+(TS^\sim)}\Omega \\ &= 0 \end{aligned}$$

- Conditions on B, e.g. e_j related with $ker(S)$

$$(e_j, Be_k) = 0$$

- Bosonic annihilation operators

$$c \sim d\hat{\Gamma}(B)$$

How to prove determinant formulae?

- n-particle expectation value

$$\omega_n(t)^2 = \omega_n(0)^2 \det(\mathbb{1} + 4t^2 AC)$$

- Bosonic vacua

$$\Omega_{d'} = a^\dagger(Tf'_d) \cdots a^\dagger(Tf_1) e^{-\frac{1}{2}\Delta^+(TS^\sim)}\Omega$$

- Exponential function of bosonic annihilation operators and creation operators

$$\omega_n(t) = (\Omega_{d'}, e^{t(c^\dagger + c)}\Omega_{d'})$$

- Evaluate $\omega_n(0)$

Bosons from Fermions

Remarks

- In $L = L^2[-\pi, \pi]$ any orthonormal system ist ok.
- An general index space L is ok not only L^2.
- Any Bogoliubov transform with general S and T is ok not only projection operators.
- Any set of commuting operators is ok not only multiplication operators.
- Any abelian subalgebra is ok not only those obtained via a Bogoliubov transform.

To do

Describe the structure of all fermionic representations of the CCR!