Fock and non-Fock states on CAR-algebras

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In the formalism of second quantization a system of fermions is described by creation and annihilation operators $a^*(f)$, $a(f)$ on the anti-symmetric Fock space $\Gamma_{\rm a}(\mathfrak{h})$ over the one-particle Hilbert space $\mathfrak{h}$. For systems confined in a finite volume, this Hilbert space description is sufficient and states of finite positive density can be represented by density matrices in $\Gamma_{\rm a}(\mathfrak{h})$. The situation changes when taking the thermodynamic (infinite volume) limit. There is no density matrix in Fock space describing a positive density state of an infinitely extended system of fermions. For such systems a more sophisticated description involving the C^*-algebra $\mathrm{CAR}(\mathfrak{h})$ is needed (see [The C^*-algebra approach]).

1 Gauge invariant states on $\mathrm{CAR}(\mathfrak{h})$

Global $U(1)$-gauge symmetry is a fundamental property of quantum mechanics. Its implementation on $\mathrm{CAR}(\mathfrak{h})$ is given by the gauge group $\mathbb{R} \ni \varphi \mapsto \vartheta^\varphi$, the group of Bogoliubov automorphisms defined by

$$\vartheta^\varphi(a^*(f)) = a^*(\mathrm{e}^{\mathrm{i}\varphi} f) = \mathrm{e}^{\mathrm{i}\varphi} a^*(f), \quad \vartheta^\varphi(a(f)) = a(\mathrm{e}^{\mathrm{i}\varphi} f) = \mathrm{e}^{-\mathrm{i}\varphi} a(f).$$

As a Banach space, $\mathrm{CAR}(\mathfrak{h})$ has a direct sum decomposition into charge sectors

$$\mathrm{CAR}(\mathfrak{h}) = \bigoplus_{n\in\mathbb{Z}} \mathrm{CAR}_n(\mathfrak{h}),$$

where $\mathrm{CAR}_n(\mathfrak{h})$ is the closed linear span of monomials of the form

$$a^*(f_1)\cdots a^*(f_j)a(g_k)\cdots a(g_1),$$

with $j-k=n$. In terms of the gauge-group one has

$$\mathrm{CAR}_n(\mathfrak{h}) = \{A \in \mathrm{CAR}(\mathfrak{h}) \,|\, \vartheta^\varphi(A) = \mathrm{e}^{\mathrm{i}n\varphi} A\}.$$

If $A \in \mathrm{CAR}_n(\mathfrak{h})$ and $B \in \mathrm{CAR}_m(\mathfrak{h})$, then $AB \in \mathrm{CAR}_{n+m}(\mathfrak{h})$, $A^* \in \mathrm{CAR}_{-n}(\mathfrak{h})$. In particular, the zero charge sector $\mathrm{CAR}_0(\mathfrak{h})$ is a C^*-subalgebra generated by I and elements of the form $a^*(f)a(g)$. Physical observables of a system of fermions are gauge invariant and hence elements of $\mathrm{CAR}_0(\mathfrak{h})$.

A state ω on $\mathrm{CAR}(\mathfrak{h})$ is gauge-invariant if $\omega \circ \vartheta^\varphi = \omega$ for all $\varphi \in \mathbb{R}$. A state ω_0 on $\mathrm{CAR}_0(\mathfrak{h})$ has a unique extension to a gauge-invariant state ω on $\mathrm{CAR}(\mathfrak{h})$, given by

$$\omega(\oplus_n A_n) = \omega_0(A_0).$$

Thus, a gauge-invariant state on $\mathrm{CAR}(\mathfrak{h})$ is completely determined by its restriction to the gauge-invariant subalgebra $\mathrm{CAR}_0(\mathfrak{h})$. When dealing with fermionic systems it is often convenient to work on the full algebra $\mathrm{CAR}(\mathfrak{h})$ and to restrict the states to be gauge-invariant.

2 Characteristic functions

Denote by $\mathcal{U}$ the group of unitaries u on $\mathfrak{h}$ such that $u - I$ is finite rank. For each $u \in \mathcal{U}$ there exist finite rank self-adjoint operators k such that

$$k = \sum_{j=1}^{n} \kappa_j f_j (f_j | \cdot), \quad u = \mathrm{e}^{\mathrm{i}k}. \tag{1}$$

Moreover, the unitary

$$U(u) = \mathrm{e}^{\mathrm{i}\sum_j \kappa_j a^*(f_j) a(f_j)} \in \mathrm{CAR}(\mathfrak{h}),$$

only depends on u, not on the particular choice of the representation (1). The Araki-Wyss characteristic function of a gauge-invariant state ω on $\mathrm{CAR}(\mathfrak{h})$ is defined as

$$\begin{array}{rccc} E: & \mathcal{U} & \to & \mathbb{C} \\ & u & \mapsto & \omega(U(u)). \end{array}$$

It satisfies

1. For any $u_1, \dots, u_N \in \mathcal{U}$ and $z_1, \dots, z_N \in \mathbb{C}$,

$$\sum_{j,k=1}^{N} E(u_j^* u_k) \bar{z}_j z_k \geq 0.$$

2. For any $u, v \in \mathcal{U}$, $f \in \mathfrak{h}$ and $\lambda \in \mathbb{R}$

$$\frac{E(u\mathrm{e}^{\mathrm{i}\lambda (f| \cdot) f} v) - E(uv)}{\mathrm{e}^{\mathrm{i}\lambda \|f\|^2} - 1},$$

is independent of λ.

Reciprocally, any function $E : \mathcal{U} \to \mathbb{C}$ satisfying the above two conditions is the characteristic function of unique gauge-invariant state ω on $\mathrm{CAR}(\mathfrak{h})$ (see [AW]).

3 Vacuum state and Fock representation

The vacuum state $\mathbf{vac}(\cdot)$ on $\mathrm{CAR}(\mathfrak{h})$ describes the system in absence of any fermion. If $\{e_i \,|\, i \in I\}$ denotes an arbitrary orthonormal basis of $\mathfrak{h}$ then $n_i = a^*(e_i)a(e_i)$ is the number of fermions in state e_i and we must have $\mathbf{vac}(\prod_{i\in J} n_i) = 0$ for any finite $J \subset I$ (note that $[n_i, n_j] = 0$). It immediately follows that the characteristic function of the vacuum state is $E_{\mathbf{vac}}(u) = 1$.

The GNS representation associated to the vacuum state is the Fock representation $(\mathcal{H}_F, \pi_F, \Omega_F)$ where $\mathcal{H}_F = \Gamma_{\mathrm{a}}(\mathfrak{h})$ is the fermionic Fock space over $\mathfrak{h}$, $\pi_F(a(f)) = a_F(f)$ is the annihilation operator on $\Gamma_{\mathrm{a}}(\mathfrak{h})$ and Ω_F is the Fock vacuum vector. For $f_i, g_j \in \mathfrak{h}$ one has

$$\mathbf{vac}(a(g_1)\cdots a(g_m)a^*(f_n)\cdots a^*(f_1)) = (a_F^*(g_m)\cdots a_F^*(g_1)\Omega_F | a_F^*(f_n)\cdots a_F^*(f_1)\Omega_F) = \delta_{nm} \det\{(g_i|f_j)\}.$$

Special features of the Fock representation are:

(i) $\pi_F(\mathrm{CAR}(\mathfrak{h}))$ is irreducible, i.e., any bounded operator on $\Gamma_{\mathrm{a}}(\mathfrak{h})$ commuting with all $a_{\mathrm{F}}^{\#}(f)$ is a multiple of the identity. Equivalently, the enveloping von Neumann algebra $\pi_F(\mathrm{CAR}(\mathfrak{h}))''$ is the C^*-algebra of all bounded operators on $\Gamma_{\mathrm{a}}(\mathfrak{h})$.

(ii) The second quantization $\Gamma(U)$ of a unitary operator U on $\mathfrak{h}$ provides a unitary implementation of the associated Bogoliubov automorphism $\gamma(a(f)) = a(Uf)$,

$$\pi_F(\gamma(a(f))) = \Gamma(U)\pi_F(a(f))\Gamma(U)^*.$$

In particular, the gauge group ϑ^t is implemented by a strongly continuous unitary group whose generator $N = \mathrm{d}\Gamma(I)$ is the number operator.

A Fock state on $\mathrm{CAR}(\mathfrak{h})$ is a state ω which is normal with respect to the vacuum state **vac**. Such a state is therefore defined by $\omega(A) = \mathrm{tr}(\rho\pi_F(A))$ where ρ is a density matrix on $\Gamma_{\mathrm{a}}(\mathfrak{h})$. The GNS representation of a Fock state ω is a direct sum of Fock representations, i.e., there exists a Hilbert space $\mathcal{K}$ such that $\mathcal{H}_\omega = \mathcal{H}_F \otimes \mathcal{K}$ and $\pi_\omega(A) = \pi_F(A) \otimes I$. Typical examples of Fock states are finite volume, grand-canonical Gibbs ensembles

$$\rho = \frac{\mathrm{e}^{-\beta(H_\Lambda - \mu N_\Lambda)}}{\mathrm{tr}(\mathrm{e}^{-\beta(H_\Lambda - \mu N_\Lambda)})},$$

for Fermi gases with stable interactions (see [BR2]). Thermodynamic limits of such states yield non-Fock states with finite density. It is usually impossible to describe explicitly the GNS representations of these infinite volume KMS states. Notable exceptions are the ideal Fermi gases which lead to the Araki-Wyss representations.

Since there exists a self-adjoint (and hence densely defined) number operator $N = \mathrm{d}\Gamma(I)$ on the Fock space $\mathcal{H}_F$, Fock states describe systems with a finite number of fermions. A number operator can be tentatively defined in the GNS representation of any state ω as follows. For any finite $J \subset I$ denote by n_J the quadratic form associated to the operator $\sum_{i\in J}\pi_\omega(n_i)$. For $\Psi \in \mathcal{H}_\omega$ set $n_\omega(\Psi) = \sup_J n_J(\Psi)$. It can be shown that n_ω is a closed, non-negative quadratic form on the domain $D_\omega = \{\Psi \in \mathcal{H}_\omega \,|\, n_\pi(\Psi) < \infty\}$. If this domain is dense then n_ω is the quadratic form of a self-adjoint number operator N_ω and the state ω is a Fock state (see [BR2] for details).

4 Anti-Fock representation

A state $\mathbf{full}(\cdot)$ describing a completely filled Fermi sea must satisfy, for any orthonormal basis $\{e_i \,|\, i \in I\}$ and any finite $J \subset I$, $\mathbf{full}(\prod_{i\in J}(1 - n_i)) = 0$. It can be obtained using the particle-hole duality. Denote by $\bar{\cdot}$ an arbitrary complex conjugation on $\mathfrak{h}$ and define the $*$-automorphism α by $\alpha(a(f)) = a^*(\bar{f})$. Since $1 - n_i = a(e_i)a^*(e_i) = \alpha(a^*(\bar{e}_i)a(\bar{e}_i))$ we can set $\mathbf{full} = \mathbf{vac} \circ \alpha$. It follows that

$$\mathbf{vac}(a(\bar{f}_1)\cdots a(\bar{f}_n)a^*(\bar{g}_m)\cdots a^*(\bar{g}_1)) = \delta_{nm}\det\{(g_i|f_j)\}.$$

For $u \in \mathcal{U}$ one has

$$\alpha(U(u)) = \det(u)U(\bar{u}),$$

hence the characteristic function of the filled Fermi sea is $E_{\mathbf{full}}(u) = \det(u)$. The corresponding GNS representation is the anti-Fock representation $(\mathcal{H}_F, \pi_{AF}, \Omega_F)$ where $\pi_{AF} = \pi_F \circ \alpha$.

If $\mathfrak{h}$ is finite dimensional then the states **vac** and **full** are mutually normal and the Fock and anti-Fock representations are equivalent. By fixing an orthonormal basis $\{e_1, \ldots, e_n\}$ and setting $a_J = \prod_{i\in J} a(e_i)$ the unitary operator defined by $UA_J^*\Omega_F = A_{I\setminus J}^*\Omega_F$ intertwines π_F and π_{AF}. If $\mathfrak{h}$ is infinite dimensional these two representations are inequivalent and **full** is not a Fock state.

5 Jordan-Wigner representation

The equivalence of the Fock and anti-Fock representations of CAR algebras over finite dimensional spaces is a consequence of a more general fact about such algebras which we discuss briefly in this last section. We refer the reader to [D] for a more detailed discussion.

If $\mathfrak{h}$ is finite dimensional then $\mathrm{CAR}(\mathfrak{h})$ is $*$-isomorphic to the full matrix algebra $\mathrm{Mat}(2^{\dim\mathfrak{h}})$. An explicit representation is provided by the Jordan-Wigner transformation described below. Since it maps fermions into quantum spins this transformation is also quite useful in many applications to statistical mechanics.

Let $\{e_1,\ldots,e_n\}$ be an orthonormal basis of $\mathfrak{h}$ and denote by $\sigma^{(1)}$, $\sigma^{(2)}$, $\sigma^{(3)}$ the Pauli matrices. On the n-fold tensor product $\mathcal{H}=\mathbb{C}^2\otimes\cdots\otimes\mathbb{C}^2\simeq\mathbb{C}^{2^n}$ define

$$\sigma_k^{(\alpha)}=I\otimes\cdots\otimes\sigma^{(\alpha)}\cdots\otimes I,$$

where $\sigma^{(\alpha)}$ acts on the k-th copy of $\mathbb{C}^2$. Clearly, this operators generate the full matrix algebra $\mathcal{B}(\mathcal{H})\simeq\mathrm{Mat}(2^n)$. One easily checks that the operators

$$a_k=\sigma_1^{(3)}\cdots\sigma_{k-1}^{(3)}(\sigma_k^{(1)}-\mathrm{i}\sigma_k^{(2)})/2,$$

satisfy $[a_k,a_l]_+=0$ and $[a_k,a_l^*]_+=\delta_{k,l}$. The Jordan-Wigner representation of $\mathrm{CAR}(\mathfrak{h})$ is defined by

$$a_{\mathrm{JW}}\left(\sum_k z_k e_k\right)=\sum_k \bar{z}_k a_k.$$

The inversion formulas

$$\sigma_k^{(3)}=2a_k^*a_k-I,\quad \sigma_k^{(1)}=\sigma_1^{(3)}\cdots\sigma_{k-1}^{(3)}(a_k+a_k^*),\quad \sigma_k^{(2)}=\mathrm{i}\sigma_1^{(3)}\cdots\sigma_{k-1}^{(3)}(a_k-a_k^*),$$

show that $\mathrm{CAR}(\mathfrak{h})$ is isomorphic to $\mathrm{Mat}(2^n)$. The Jordan–Wigner representation plays for fermions the same role as the Schrödinger representation of the CCR: If $\dim\mathfrak{h}<\infty$ then any irreducible representation of $\mathrm{CAR}(\mathfrak{h})$ is equivalent to the Jordan–Wigner representation.

References

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