NONCOMMUTATIVE FERMI SURFACES

Jean BELLISSARD[1 2]
Université Paul Sabatier, Toulouse
MSRI
&
Institut Universitaire de France

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Collaboration:

D. SPEHNER *(Pontificia Universidad Catolica de Chile)*

[1]I.R.S.A.M.C., Université Paul Sabatier, 118, route de Narbonne, Toulouse Cedex 04, France
[2]e-mail: jeanbel@irsamc2.ups-tlse.fr

I - What is a FERMI Surface ?

Periodicity :

1. Periodic perfect crystal.
   Interactions between electrons are ignored.

2. Schrödinger's equation:

$$H = -\frac{\hbar^2}{2m}\Delta + V(x) \quad \text{on} \quad L^2(\mathbb{R}^d)$$

3. Period group $\mathbb{G}$ with:

$$V(x+a) = V(x) \qquad \forall a \in \mathbb{G}$$

4. BRAVAIS cell $\quad \mathbb{V} = \mathbb{R}^d/\mathbb{G}$

   BRILLOUIN zone $\quad \mathbb{B} = \hat{\mathbb{R}}^d/\mathbb{G}^{\perp} \simeq \mathbb{G}^*$

Bloch Theorem ('28):

Theorem 1 (Bloch)

1.

$$L^2(\mathbb{R}^d) \simeq \int_{\mathbb{B}}^{\oplus} \frac{d^d k}{|\mathbb{B}|}\, \mathcal{H}_k \qquad \mathcal{H}_k \simeq L^2(\mathbb{T}^d)$$

$$H \simeq \int_{\mathbb{B}}^{\oplus} \frac{d^d k}{|\mathbb{B}|}\, H_k \qquad H_k = \frac{1}{2m}\left(\frac{\hbar}{\imath}\vec{\nabla} + \vec{k}\right)^2 + V$$

with periodic boundary conditions.

2. H_k *has compact resolvent. For generic* V*'s, the eigenvalues* $\left(E_j(k)\right)_{j=0}^{\infty}$ *have multiplicity one.*

3. If $E_j(k)$ *simple* $\forall k \in \mathbb{B}$, $k \in \mathbb{B} \mapsto E_j(k) \in \mathbb{R}$ *is analytic.*

Fermi level :

1. The *density of states* (DOS) is the number of eigenstates of H per unit volume:

$$d\mathcal{N}(E) = \sum_j \int_{\mathbb{B}} \frac{d^d k}{|\mathbb{B}|} \; \delta(E - E_j(k))$$

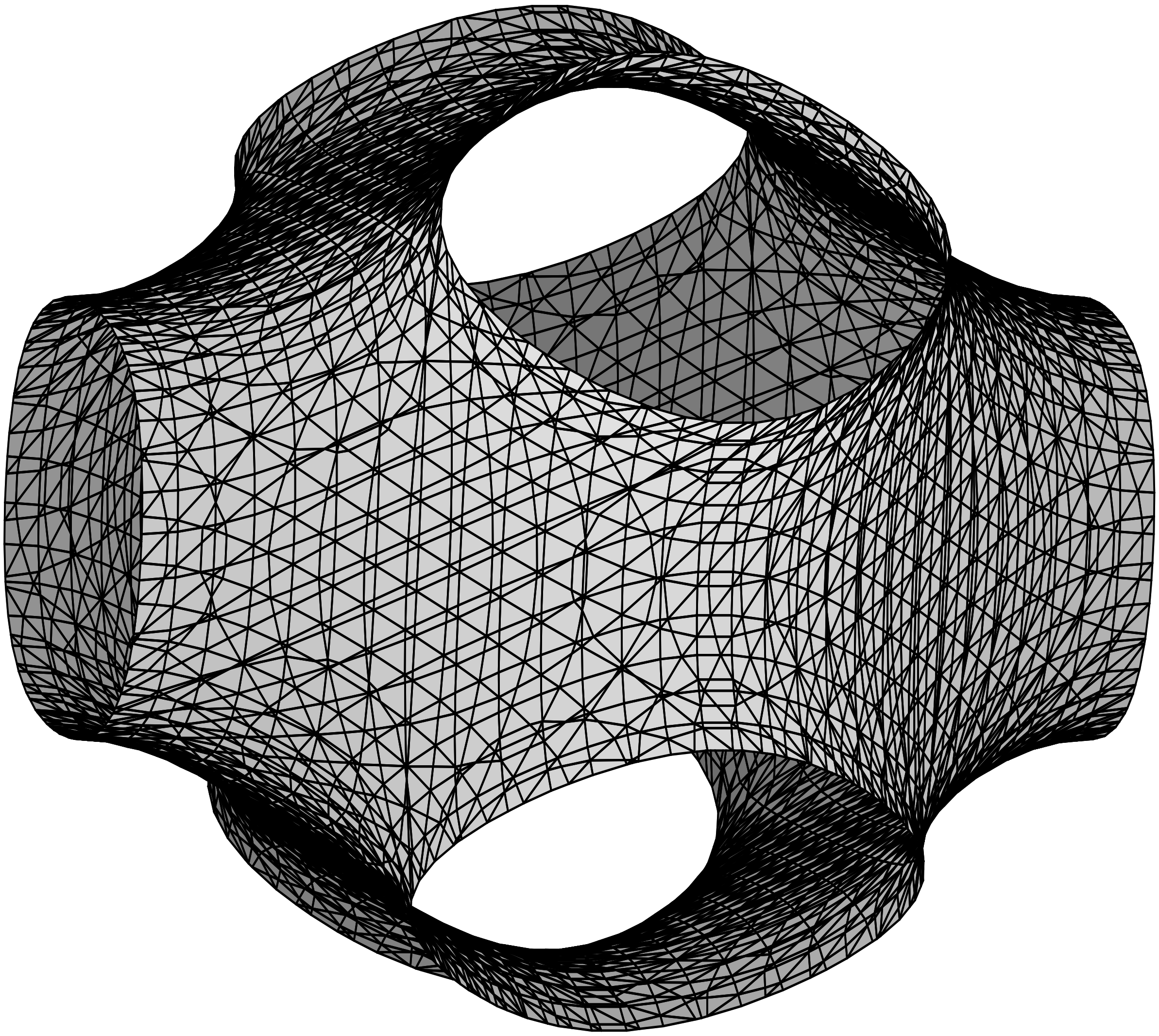
2. The *electron density* n_e is the number of electrons per unit volume.

3. Electrons are *fermions*: one electron per state. Thus, *in their groundstate*, they fill all states up to the energy E_F such that

$$\int_{-\infty}^{E_F} d\mathcal{N}(E) \; = \; n_e$$

4. The *Fermi surface* is:

$$\Sigma_F = \bigcup_j \; \{k \in \mathbb{B}\,; \; E_j(k) = E_F\}$$



- The Fermi surface for copper-

Thermal Fluctuations :

1. At non zero temperature ($\beta < \infty$), electronic states are partially occupied according to:

$$f_{\beta,\mu} = \frac{1}{(1 + e^{\beta(E-\mu)})}$$

Fermi Dirac distribution

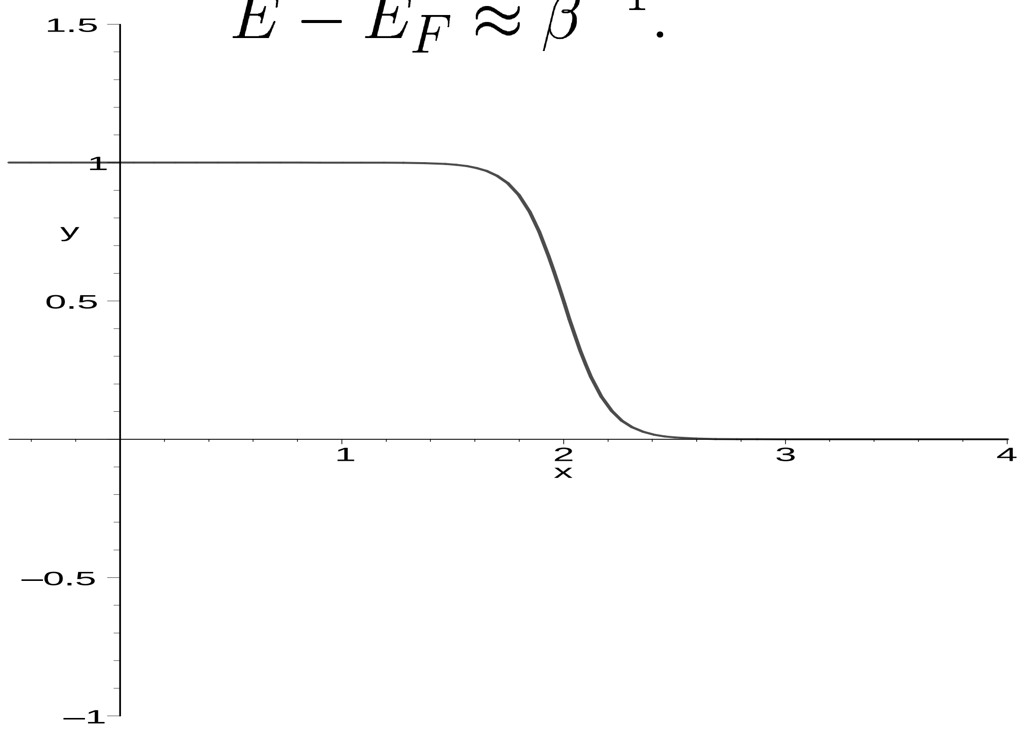
where μ is fixed by

$$\int_{\mathbb{R}} d\mathcal{N}(E)\, f_{\beta,\mu}(E) = n_e$$

(so that $E_F = \lim_{\beta\uparrow\infty} \mu(\beta, n_e)$.)

2. Carrying current states are those for which

$$E - E_F \approx \beta^{-1}.$$



Aperiodicity & Interactions:

1. The Fermi surface is well-defined for independent electrons in a perfect crystal *(periodic solid)*.

2. Can one extend this notion for *aperiodic solids* ? Then the Brillouin zone becomes a *noncommutative manifold*.

3. Can one also take interactions into account ?

4. How does one describe the electrons, the phonons, the other degrees of freedom ?

5. Is there an analog of the Fermi surface if aperiodicity and interactions are considered together ?

II - Electrons & Phonons in Aperiodic Solids

Noncommutative BRILLOUIN zone:

1. Ideal atomic positions make up a point set $\mathcal{L} \subset \mathbb{R}^d$ which is *uniformly discrete*.
2. A suitable closure of the family $\{\mathcal{L} + a\,;\, a \in \mathbb{R}^d\}$ gives a metrizable compact space Ω endowed with a $\mathbb{R}^d$-action. The dynamical system $(\Omega, \mathbb{R}^d, \tau)$ is called the *Hull*.
3. An element $\omega \in \Omega$ defines a limiting point set $\mathcal{L}_\omega$ which is uniformly discrete.
4. The *canonical transversal* X is the closed subset of points ω such that $0 \in \mathcal{L}_\omega$.
5. Let Γ be the subgroupoid of $\Omega \rtimes_\tau \mathbb{R}^d$ defined by X. Then $\Gamma^{(0)} = X$ and for $\omega \in X$ the r-fiber is given by $\Gamma^\omega = \mathcal{L}_\omega$.
6. $C^*(\Gamma)$ plays the rôle of continuous functions on the *noncommutative Brillouin zone.*

One-Electron Dynamics:

1. Independent electrons are described by the *Schrödinger Hamiltonian* acting on $L^2(\mathbb{R}^d)$. However, only those electrons with energies near E_F matters.

2. The effective Hamiltonian is a matrix $H_\omega(x, y)$ indexed by points $x, y \in \mathcal{L}_\omega$, with fast decrease in $x - y$. It then defines an operator on $\ell^2(\mathcal{L}_\omega)$.

3. Covariance: if $(\omega, a) \in \Gamma$,
$$H_{\mathcal{T}^{-a}\omega}(x - a, y - a) = H_\omega(x, y)$$
so that $h(\omega, x) = H_\omega(0, x) \Longrightarrow h \in C^*(\Gamma)$.

4. If spin or orbitals degrees of freedom are taken into account, the Hamiltonian acts on $\ell^2(\mathcal{L}_\omega) \otimes \mathbb{C}^N$ for some N instead. Thus $h \in C^*(\Gamma) \otimes M_N(\mathbb{C})$.

N-Electron Dynamics:

1. For a given $\omega \in \Omega$, the fermion creation-annihilation operators $f^{\dagger}_{(\omega,x),\sigma}$, $f_{(\omega,x),\sigma}$ are indexed by sites in $\mathcal{L}_\omega$ and by spin or orbital indices.

2. They fulfill the *canonical anticommutation relation* (CAR):

$$f_{(\omega,x),\sigma}\, f^{\dagger}_{(\omega,y),\sigma'} + f^{\dagger}_{(\omega,y),\sigma'}\, f_{(\omega,x),\sigma} = \delta_{x,y}\delta_{\sigma,\sigma'}$$

3. They generate a field of CAR-algebra $\mathfrak{E}_\omega$.

4. For $\gamma : \omega \mapsto \omega' \in \Gamma$, there is a *-isomorphism $\epsilon_\gamma : \mathfrak{E}_\omega \mapsto \mathfrak{E}_{\omega'}$ defined by

$$\epsilon_\gamma\, f_{(\omega,x),\sigma} = f_{\gamma\circ(\omega,x),\sigma}$$

   satisfying $\epsilon_\gamma \epsilon_{\gamma'} = \epsilon_{\gamma\circ\gamma'}$ if the arrows are composable, and $\epsilon_\gamma^{-1} = \epsilon_{\gamma^{-1}}$.

5. **Theorem 2** *The pair $(\mathfrak{E}, \epsilon)$ defined above, is a continuous covariant field of C^*-algebras .*

N-Electron Hamiltonian:

1. The second quantized of the one-electron Hamiltonian is:

$$(H_{el})_\omega = \sum_{x,y \in \mathcal{L}_\omega, \sigma, \sigma'} H_\omega(x,y)_{\sigma,\sigma'} f^\dagger_{(\omega,x),\sigma} f_{(\omega,y),\sigma'}$$

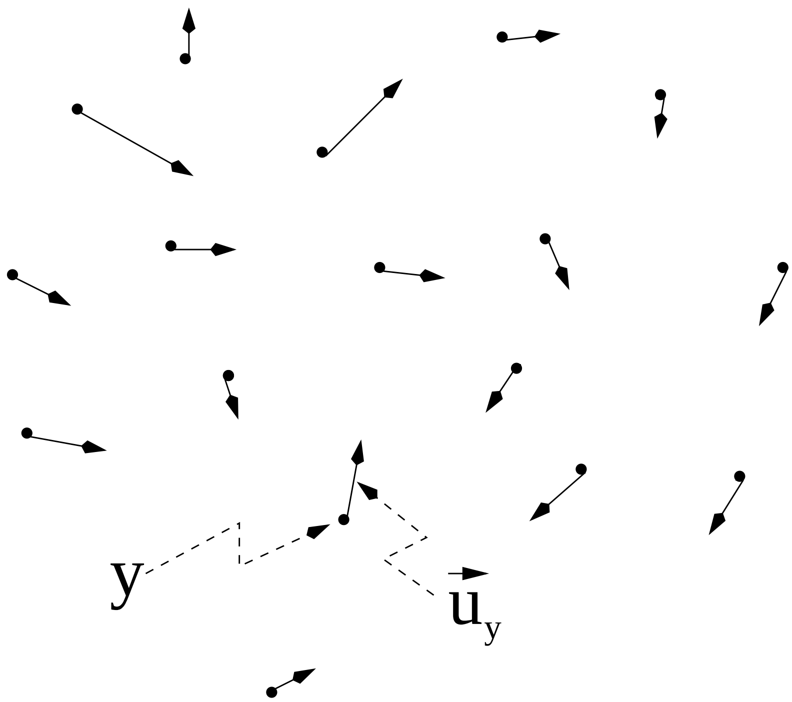
2. Electrons interact: a typical model for interaction is:

$$(H_{e-e})_\omega = \sum_{x,y} V(x-y) n_{(\omega,x)} n_{(\omega,y)}$$

   where $n_{(\omega,x)} = \sum_\sigma f^\dagger_{(\omega,x),\sigma} f_{(\omega,y),\sigma}$

3. The electronic Hamiltonian is then $H_{el} + H_{e-e}$.

Phonons Dynamics:



1. Phonons are acoustic waves produced by small displacements of the atomic nuclei.
2. These waves are polarized with d-directions of polarization: $d-1$ are *transverse* one is *longitudinal*.
3. The nuclei motion is approximatively harmonic and quantized according to the *Bose-Einstein* statistics.
4. The charged nuclei interact with electrons, leading to an *electron-phonon interaction*.

The Harmonic Approximation:

1. If the nuclei motion is harmonic, the classical equations of motion are:

$$M_{(\omega,x)} \frac{d^2 \vec{u}_{(\omega,x)}}{dt^2} = \sum_{x \neq y \in \mathcal{L}_\omega} K_\omega(x,y) \left(\vec{u}_{(\omega,y)} - \vec{u}_{(\omega,x)}\right)$$

   where $M_{(\omega,x)}$ is the mass of the nucleus located at x, $\vec{u}_{(\omega,x)}$ is its classical displacement vector and $K_\omega(x,y)$ is the matrix of *spring constants*.

2. $K_\omega(x,y)$ decays fast in $x-y$, uniformly in ω..

3. Covariance gives

$$M_{(\omega,x)} = m(\tau^{-x}\omega) \qquad K_\omega(x,y) = k(\tau^{-x}\omega, y-x)$$

   thus $m \in \mathcal{C}(X) \subset C^*(\Gamma)$, $k \in C^*(\Gamma) \otimes M_d(\mathbb{C})$.

4. Let $\hat{\Omega} \in C^*(\Gamma)$ be defined by (for $\vec{s}_x \in \mathbb{C}^d$).

$$\sum_{x,y} \frac{\vec{s}_x^{\,*}}{\sqrt{M_{\omega,x}}} \left(\hat{\Omega}_\omega^2\right)_{x,y} \frac{\vec{s}_y}{\sqrt{M_{\omega,x}}} = \sum_{x \neq y} (\vec{s}_x - \vec{s}_y)^* K_\omega(x,y) (\vec{s}_x - \vec{s}_y)$$

   Then $\hat{\Omega}^\alpha(\omega,x)_{\rho,\rho'} \geq 0$ if $\alpha < 2$.

The Phonon Hamiltonian:

1. The variables $\vec{u}_{(\omega,x)}$ and $\vec{v}_{(\omega,x)} = M_{(\omega,x)} d\vec{u}_{(\omega,x)}/dt$ can be quantized through (here $\rho = 1, \cdots, d$) :

$$\hat{u}_{\omega,x,\rho} = \sqrt{\frac{\hbar}{2M_{(\omega,x)}}} \sum_{y,\rho'} (\hat{\Omega}_\omega^{-1/2})(x,y)_{\rho,\rho'} \left(b_{(\omega,y),\rho'} + b^\dagger_{(\omega,y),\rho'} \right)$$

$$\hat{v}_{\omega,x,\rho} = \sqrt{\frac{\hbar M_{(\omega,x)}}{2}} \sum_{y,\rho'} (\hat{\Omega}_\omega^{-1/2})(x,y)_{\rho,\rho'} \left(\frac{b_{(\omega,y),\rho'} - b^\dagger_{(\omega,y),\rho'}}{\imath} \right)$$

where the $b, b^\dagger$'s are annihilation-creation operators for bosons.

2. The *harmonic phonon Hamiltonian* is

$$(H_{ph})_\omega = \sum_{x,y \in \mathcal{L}_\omega} \sum_\rho (\hat{\Omega}_\omega^{-1/2})(x,y)_{\rho,\rho'} \, b^\dagger_{(\omega,x),\rho} \, b_{(\omega,y),\rho'}$$

$$= \sum_x \frac{\vec{v}^{\,2}_{(\omega,x)}}{2M_{(\omega,x)}} + \sum_{x,y} \langle \vec{u}_{(\omega,x)} - \vec{u}_{(\omega,y)} | K_\omega(x,y) | \vec{u}_{(\omega,x)} - \vec{u}_{(\omega,y)} \rangle$$

3. Anharmonic terms, higher degree polynomials in the $b, b^\dagger$'s, may be added if necessary.

N-Phonons Dynamics:

1. For a given $\omega \in \Omega$, the boson creation-annihilation operators $b^{\dagger}_{(\omega,x),\rho}$, $b_{(\omega,x),\rho}$ are indexed by sites in $\mathcal{L}_\omega$ and by polarization indices.

2. They fulfill the *canonical commutation relation* (CCR):

$$b_{(\omega,x),\rho}\, b^{\dagger}_{(\omega,y),\rho'} - b^{\dagger}_{(\omega,y),\rho'}\, b_{(\omega,x),\rho} = \delta_{x,y}\delta_{\rho,\rho'}$$

3. They generate a field of CCR-algebra $\mathfrak{P}_\omega$.

4. For $\gamma : \omega \mapsto \omega' \in \Gamma$, there is a *-isomorphism $\phi_\gamma : \mathfrak{P}_\omega \mapsto \mathfrak{P}_{\omega'}$ defined by

$$\phi_\gamma\, b_{(\omega,x),\rho} = b_{\gamma\circ(\omega,x),\rho}$$

satisfying $\phi_\gamma \phi_{\gamma'} = \phi_{\gamma\circ\gamma'}$, if the arrows are composable, and $\phi_\gamma^{-1} = \phi_{\gamma^{-1}}$.

5. **Theorem 3** *The field* $(\mathfrak{P}, \phi)$ *defined above, as well as* $(\mathfrak{E} \otimes \mathfrak{P}, \epsilon \otimes \phi)$ *are continuous covariant fields of* C^**-algebras .*

The Global Dynamic:

1. The electron-phonon Hamiltonian is then given by

$$H = H_{el} + H_{e-e} + H_{ph} + H_{e-\phi}$$

where $H_{e-\phi}$ is the electron-phonon interaction.

2. A typical example for $H_{e-\phi}$ is (FRÖHLICH's model):

$$(H_{e-\phi})_\omega = \sum_{x,y \in \mathcal{L}_\omega} \lambda_{\omega,\rho}(x,y)\, n_{(\omega,x)}\, \hat{u}_{x,\rho}$$

3. The previous expressions define selfadjoint operators only whenever the sums are restricted to a finite volume. However, the infinite volume limit exists as a derivation on $\mathfrak{A} = \mathfrak{E} \otimes \mathfrak{P}$:

Theorem 4 *The total Hamiltonian H_ω defines a one-parameter group of *-automorphisms η^t_ω on $\mathfrak{A}_\omega$ that is continuous in ω and covariant, namely, if $\gamma : \omega \mapsto \omega'$ and if $\alpha = \epsilon \otimes \phi$:*

$$\alpha(\gamma)\ \eta^t_\omega\ \alpha(\gamma)^{-1}\ =\ \eta^t_{\omega'}$$

III - Ground States Bimodules

Full Observable Algebra :

1. The covariance of $(\mathfrak{A}, \alpha) = (\mathfrak{E} \otimes \mathfrak{P}, \epsilon \otimes \phi)$ means that the groupoid Γ acts on it, so that the crossed product $\mathfrak{B} = \mathfrak{A} \rtimes_\alpha \Gamma$ is well-defined *(Renault, '86)*.
2. $\mathfrak{B}$ is generated by continuous funtions $\gamma \in \Gamma \mapsto A(\gamma) \in \mathfrak{A}_\omega$, if $\omega = r(\gamma)$, with compact support.
3. The product is given by
$$(AB)(\gamma) = \sum_{\gamma' \in \Gamma^\omega} A(\gamma')\alpha(\gamma')B(\gamma'^{-1} \circ \gamma)$$
4. the adjoint by:
$$A^*(\gamma) = \alpha(\gamma)A(\gamma^{-1})^*$$
5. The (reduced) norm is obtained through covariant representations.
6. $\mathfrak{B}$ is also a $C^*(\Gamma)$-bimodule.

Covariant States & GNS Representation:

1. A covariant state on $\mathfrak{A}$ is continuous a family Φ_ω of states on $\mathfrak{A}_\omega$ such that

$$\Phi_\omega \circ \alpha(\gamma) = \Phi_{\omega'} \quad \textit{if} \quad \gamma : \omega' \mapsto \omega$$

2. A Hilbert C^*-module structure over $C^*(\Gamma)$ is defined on $\mathfrak{B}$ by:

$$\langle A|B\rangle(\gamma) = \Phi_\omega\left(A^* B(\gamma)\right)$$

   After quotienting and completion we get a Hilbert C^*-module $\mathcal{F}$.

3. In particular
   (a) $\langle A|B\rangle \in C^*(\Gamma)$,
   (b) If $h \in C^*(\Gamma)$ then $\langle A|Bh\rangle = \langle A|B\rangle h$.
   (c) $\langle A|B\rangle^* = \langle B|A\rangle$.
   (d) $\langle A|CB\rangle = \langle C^* A|B\rangle$

4. So that the left multiplication by an element of $\mathfrak{B}$ defines an endomorphisms of $\mathcal{F}$, giving rise to the *GNS representation* of $\mathfrak{B}$ in $\mathcal{F}$.

Ground States:

1. If Φ is η-invariant, η^t is implemented by a one parameter group $U(t)$ of unitary endomorphisms of $\mathcal{F}$:
$$\langle A|U(t)B\rangle = \langle A|\eta^t(B)\rangle$$
2. If, in addition, Φ is a *ground state* for η, then the generator $H = -\imath U(t)^{-1}dU/dt$ is *positive*, namely
$$\langle A|HA\rangle \geq 0 \qquad\qquad \forall A \in \mathcal{F}$$
3. This construction applies to the case of the electron-phonon dynamics in an aperiodic solid: a ground state is specified by the Fermi level E_F. The Hilbert C^*-module $\mathcal{F}_F$ obtained in this way, plays the rôle of a fiber bundle over the Noncommutative Brillouin zone defined by $C^*(\Gamma)$, fixing somehow the geometry of the Fermi surface.

We propose therefore the following definition:

Definition 1 *The Noncommutative Fermi surface associated to the dynamics defined by the total Hamiltonian H, and to the Fermi energy E_F is the NC fiber bundle above the NC Brillouin zone associated with the Hilbert C^*-module $\mathcal{F}_F$ constructed above.*

IV - Conclusion

1. Quantization of interacting electrons and phonons in an aperiodic crystal can be done through a continuous field $\mathfrak{A}$ of CCR-CAR algebras over the canonical transversal of the Hull of the solid.
2. This field is covariant with respect to the groupoid Γ of the transversal. A crossed product with Γ leads to the full observable algebra $\mathfrak{B}$.
3. A covariant continuous family of states over $\mathfrak{A}$ gives a GNS representation through a Hilbert C^*-module $\mathcal{F}$ over Γ.
4. The electron-phonon Hamiltonian, defines a one-parameter group of automorphisms of $\mathfrak{B}$. Invariant states leads to a one-parameter group of unitary endomorphisms of $\mathcal{F}$. The generator is positive for a ground state.
5. For ground states with given electron density, $\mathcal{F}$ characterizes the geometry of the Fermi surface.