Contact interactions II; Gross-Pitaevskii equation, Bose-Einstein condensate, Fermi sea

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Abstract In Dell'Antonio (Eur Phys J Plus 13:1–20, 2021), we explored the possibility to analyse contact interaction in Quantum Mechanics using a variational tool, Gamma Convergence. Here, we extend the analysis in Dell'Antonio (Eur Phys J Plus 13:1–20, 2021) of joint weak contact of three particles to the non-relativistic case in which the free one particle Hamiltonian is $H_0 = -\frac{\Delta}{2M}$. We derive the Gross-Pitaevskii equation for a system of three particles in joint weak contact. We then define and study strong contact and show that the Gross-Pitaevskii equation is *also* the variational equation for the energy of the Bose-Einstein condensate (strong contact in a four-particle system). We add some comments on Bogoliubov's theory. In the second part, we use the non-relativistic Pauli equation and weak contact to derive the spectrum of the conduction electrons in an infinite crystal. We prove that the spectrum is pure point with multiplicity two and eigenvalues that scale as $\frac{1}{\log n}$.

1 Introduction

In [1], we introduced *contact interactions*, self-adjoint extensions of the symmetric operator H_0^0 , the free three-body Hamiltonian restricted to functions that have support away from the "contact manifold" $\Gamma \equiv x_i - x_j = 0 \ i \neq j, \ x_j \in \mathbb{R}^3$.

In [1], we used as free one-body Hamiltonian the operator $H_0 = -\sum_{i=1}^3 (-\Delta_i + m) \ m > 0$; we called this choice *semi-relativistic*.

Here, we will consider the case $H_0 = -\sum_{i=1}^3 (-\frac{\Delta_i}{2M}) \ M > 0$ *non-relativistic*.

The Hamiltonian of weak contact is a self-adjoint extensions of the symmetric operator H_0^0 . Its domain contains functions that take a finite value at the "contact manifold" Γ .

For a two-body system in $\mathbb{R}^3$, this condition implies the presence of a zero energy resonance.

For one body on the positive real line, the self-adjoint extension would be a Friedrichs extension [10].

In our case, the construction is more difficult and requires a new approach. The difficulty lies in the fact that the "interaction potential" is only defined as a quadratic form.

Weak contact in $\mathbb{R}^3$ with a particles of infinite mass is the *point interaction* introduced by S.Albeverio [12]

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We consider the three-body problem and introduce, as intermediate step, a map to a space of more singular functions; the map is *mixing* (it does not preserve the particle structure) and *fractioning* (the new space is a space of more singular functions).

For "historical" reasons, we call this space *Minlos space* $\mathcal{M}$ [11] and call the map *Krein map* $\mathcal{K}$.

In the extended space $\mathcal{M}$, the system is described by a well-ordered one parameter family of self-adjoint operators. Inverting the map changes the metric topology and gives a well ordered family of weakly closed symmetric quadratic forms.

We make use of a variational tool, Gamma convergence, to extract the lowest quadratic form; this form can be closed strongly and provides a self-adjoint operator, the Hamiltonian of the system.

This system of three particles in mutual weak contact is described by the Gross–Pitaevskii cubic focusing equation and by the corresponding Gross–Pitaevskii energy functional $\int (|\nabla \phi(x)|^2 - |\phi|^4) dx$. This functional has an essential singularity at the origin (solitons)

The Hamiltonian of strong contact is defined as the self-adjoint extension of the free Hamiltonian H_0^0 that has in its domain functions that have a cusp at contact. The shape of the cusp determines the extension.

In a four-particles system, this Hamiltonian describes the Bose–Einstein condensate. We shall see that the Gross–Pitaevskii equation is *also* the variational equation for the energy functional of this condensate.

This functional is formally identical to the G-P functional, but it has no singularity at zero energy.

The B.E. condensate can be described as a collection of sets made of two pairs of identical bosons; the particles in each pair are in *strong* contact, and the barycenters of two pairs of particles are in strong contact.

The "condensate" is held together by a potential of class $L^1(R^3) \cap L^2(R^3)$; since the contact interaction is supported by a set of measure zero, this binding potential can be introduced without affecting the structure of the system (because this additional potential can be taken to vanish at contact, a set of measure zero).

We add a few remarks on Bogoliubov theory [13]

In the second part of the paper, we use (weak) contact interaction to study the spectrum of the conduction electrons in an infinite crystal. For the crystal, we choose a cubic lattice.

The electrons are spin $\frac{1}{2}$ particles in R^3 that satisfy the Pauli equation with Hamiltonian $H = \sigma \cdot \nabla$. They interact with the vertices of the Bloch cells through weak contact.

Due to the scaling properties in space of the Coulomb potential, the force exerted by the nuclei of the entire crystal on a conduction electron is equivalent to weak contact at the vertices of a Bloch cell.

We use the Pauli equation and weak contact to prove that the energy spectrum of the conduction electrons is pure point with eigenvalues that scale as $\frac{1}{\log n}$ and have multiplicity two. (see [1])

The same result can be obtained using the *non-relativistic* Schrödinger equation.

Electrons are fermions, and no two of them can occupy the same state. The *Fermi sea* is the state in which all bound states are occupied.

The structure of the spectrum gives an equilibrium state at very low temperature in which the energy levels are equally spaced; this implies quantisation of the linear response.

2 Contact interactions

In [1], we introduced strong and weak contact interactions as self-adjoint extensions of the free Hamiltonian $H_0 = \sum_1^3 (-\Delta_i + m_i)$ restricted to functions that have support away from the contact manifold $\Gamma \equiv x_i - x_j = 0$, $x_i \in \mathbb{R}^3$.

We consider first weak contact; we take as free Hamiltonian the non-relativistic Hamiltonian. $H_0 = \frac{\Delta}{2m}$; in the following, we choose units in which $m = 2$.

Weak contact is a self-adjoint extension of H_0^0 , the free Hamiltonian of the three particle system restricted to functions that have support away from Γ .

The extension has in its domain functions that take a finite value c at Γ .

This boundary condition implies the presence of a zero energy resonance for the two-particles system [12]

To construct this self-adjoint extension in the case $m > 0$, we have followed in [1] the following prescription.

For a three-body system, we introduce a map (the Krein map $\mathcal{K}$) from $L^2(\mathbb{R}^9)$ to a space $\mathcal{M}$ (Milnos space [11]) of more singular functions; the map is mixing (it is not diagonal in the three-body channels) and fractioning (the new space contains functions that singular at Γ).

By duality in $\mathcal{M}$, the Hamiltonian is more regular.

In $\mathcal{M}$, the kinetic energy and the potential energy have at Γ the same singularity but with opposite sign.

The system is represented therefore [3,4] in $\mathcal{M}$ by a family of self-adjoint operators. Each of them has an infinite number of zero eigenvalues that converge to zero at the rate $c \frac{1}{\sqrt{n}}$.

Inverting the map results, due to the change in metric topology, in an ordered family of weakly quadratic forms which are strictly convex (the contact interaction is rotation invariant).

Since there are no zero energy resonances, these forms are contained in a set that is compact for a Sobolev topology.

One can now use by Gamma convergence [2], a variational process to extract the infimum form.

By a result of Kato [5], the infimum can be closed strongly and is the self-adjoint Hamiltonian of the system

The operator we obtain is nonnegative and has an infinite number of zero energy resonances (i.e. an essential singularity at the bottom of the spectrum).

We proved in [1] that the contact Hamiltonian is the limit *in strong resolvent convergence* of a sequence of Hamiltonians with two-body potentials that scale as $V_\epsilon(x) = \frac{1}{\epsilon^2} V(\frac{x}{\epsilon})$, so that they have constant L^1 norm.

The quadratic form of the contact Hamiltonian is the lower bound of the quadratic forms associated with the sequence of potentials.

One has strong resolvent convergence of the Hamiltonians *but not operator convergence*.

In the strong operator topology, *there are sequence of the approximated Hamiltonians that diverge*.

The method is non-perturbative.

Remark We have analysed in [1] the case of strong contact. We have seen there that strong contact of a particle with two identical ones leads to the Efimov effect in low energy physics and to the binding of the Helium atom.

3 The Krein map, case $H_0 = \sum_{i=1}^3 (-\Delta_i + m)$ $m > 0$. [1]

For convenience of the reader, we recall the main steps taken in [1] to associate a self-adjoint operator to weak contact.

The Krein map $\mathcal{K}$ is an invertible map from $L^2(R^9)$ to a space $\mathcal{M}$ of more singular functions; both the map and its inverse are positivity preserving. We call this space *Minlos space* for historical reasons [11].

Let H_0 be the free Hamiltonian of the three particle system (for convenience, we take them identical).

The "perturbation" is supported by the contact manifold Γ .

It is the limit as $\epsilon \rightarrow 0$ in the weak topology of a sequence of negative potentials that scale as $\frac{1}{\epsilon^2} V(\frac{x_i - x_j}{\epsilon})$ $i, j = 1, 2, 3$ $V \in L^1(R^3)$.

The limit is a quadratic form W .

It is easy to see that as quadratic forms H_0 and W commute

The map acts in the same way on the kinetic energy and on the potential.

Through the Krein map, the quadratic W is mapped into $H_0^{-\frac{1}{4}} W H_0^{-\frac{1}{4}} \equiv H_i$,

The operator H_0 is mapped into the operator $H_0^{-\frac{1}{4}} H_0 H_0^{-\frac{1}{4}} = H_0^{\frac{1}{2}}$.

The map is mixing because it does not preserve the channel structure and fractioning because it maps to a space of more singular functions.

This strongly suggests the use of Gamma Convergence [2], a variational method introduced by de Giorgi in the theory of composite media.

The form $H_0^{-\frac{1}{4}} W H_0^{-\frac{1}{4}}$ can be closed strongly in $\mathcal{M}$ and defines a self-adjoint operator H_{int} .

In the space $\mathcal{M}$, the two operators $H_0^{\frac{1}{2}}$ and H_{int} have kernels that have opposite signs and the same divergence $\frac{1}{\sqrt{d}}$ where d is for each pair the distance from the centre.

Therefore [3,4] (fall to the centre), there is a denumerable well-ordered collection of self-adjoint operators H_α with parameter $\alpha \in \mathbb{Z}$.

Each operator in the family has an infinite set of eigenvalues that scale as $\lambda_n = -c(\alpha)j \frac{1}{\sqrt{n}}$, $c(\alpha) < 0$ where j is angular momentum.

Returning to $L^2(R^9)$ through the action of $H_0^{\frac{1}{2}}$, one has a one parameter family of ordered quadratic forms Q_α , $\alpha \in \mathbb{N}$ uniformly bounded below; they are *only weakly closed* due to the change in the metric topology. They are strictly convex.

As remarked above, the fact that the Krein map is mixing and fractioning suggests the use of Gamma convergence [2] a variational method introduced by E.de Giorgi and commonly used in the theory of composite materials.

Gamma convergence selects the infimum of the ordered sequence of quadratic forms.

The quadratic forms are uniformly bounded below and lie in a compact domain of a topological space Y (there are no zero energy resonances).

The Gamma limit $F(y)$ is the quadratic form defined by the relations

$$\forall y \in Y, y_n \rightarrow y; F(y) = \liminf F(y_n) \quad \forall x \in Y_n \quad \forall \{x_n\} : F(x) \leq \limsup F_n(x_n) \quad (1)$$

The first condition implies that $F(y)$ is a common lower bound for the function F_n , and the second implies that this lower bound is optimal.

The condition for the existence of the Gamma limit is that the sequence be contained in a compact set for the topology of Y (so that a Palais–Smale convergent sequence exists).

In our case, the topology of Y is the Frechet topology defined by Sobolev semi-norms and compactness follows from the absence of resonances in the spectrum.

Therefore, in our case the Gamma limit of the quadratic forms exists and is bounded below. It is strictly convex.

By a theorem of T.Kato [5], the limit form admits strong closure in a Sobolev norm and defines therefore a self-adjoint operator.

This self-adjoint operator is the Hamiltonian of joint weak contact of three identical particles.

We proved in [1] that it has an infinite set of negative eigenvalues that if $m = 0$ scale as $\lambda_n = -\gamma(\alpha) \frac{1}{|\log n|}$.

Notice that the procedure we have followed to find this operator is *variational and non-perturbative*.

4 The non-relativistic case $m = 0$

For a system of three identical particles in mutual weak contact interaction, we derived in [1] an equation that differs from the Gross–Pitaevskii equation

$$i \partial_t \phi(x, t) = -\Delta \phi(x, t) - c \phi^3(x, t) \quad x \in \mathbb{R}^3 \quad c > 0 \quad (2)$$

by the constant m that enters in our choice of $H_0 = -\Delta + m$.

We want to extend our results to the Hamiltonian $H_0^{n,r} = -\frac{\Delta}{2M}$, $M = \frac{1}{2}$ (i.e. $m=0$).

This two-body contact Hamiltonian has a zero energy resonance.

Setting $m = 0$ (non-relativistic case) may give problems in the definition of the Krein map because the Hamiltonian is not strictly positive.

We shall prove (Lemma 1 below) that the Krein map is well defined also for $m = 0$.

One has still a well-ordered family of self-adjoint operators.

Inverting the Krein map, one has again a well-ordered family of weakly closed quadratic forms.

By Gamma convergence also in the case $m = 0$, we can extract the infimum form; this form can be closed strongly and defines a self-adjoint operator H .

Since the Hamiltonians H_ϵ with the approximating potentials V^ϵ form a decreasing sequence, for any $\epsilon > 0$ one has $H_\epsilon > H$ and since compactness holds the Hamiltonian of weak joint contact is the limit in strong resolvent convergence sense of the Hamiltonians with two body potential $V^\epsilon(x_i - x_j)$, $x_i \in \mathbb{R}^3$ that scale as $V^\epsilon(x_i - x_j) = \frac{1}{\epsilon^2} V(\frac{x_i - x_j}{\epsilon})$.

Strong resolvent convergence implies convergence of spectra. There is no operator convergence and no rate of convergence can be found in the parameter ϵ . In the case $m = 0$, there is an essential singularity at the bottom of the spectrum.

Remark The choice $m > 0$ is made in [1] to assure that the Krein map is well defined. In Lemma 1, we will prove that for a three-body system the Krein map is well defined also per $m = 0$

The singularities are the same, and therefore, Weyl's criterion applies.

Therefore, the analysis in $\mathcal{M}$ follows for $m = 0$ exactly the lines followed in [1] for the case $m > 0$.

Notice that in [1] we have written the Ginsburg-Landau functional case for $m = 0$.

Indeed, the interaction between Cooper pairs is non-relativistic, repulsive and has a resonances is at zero energy (infinite scattering length).

We prove now

Lemma 1 *For a three particle system in mutual weak contact, the Krein map is well defined also for $m = 0$ (non-relativistic three-body Hamiltonian).*

Proof If $m = 0$, the short distance structure of the three-body Hamiltonian is not changed. There may be now an infrared divergence.

We will prove that for three body joint weak contact there is no infrared divergence, and the Krein map is well defined also if $m = 0$.

Let δ be a positive parameter and define a family of "Krein maps" as

$$H_\epsilon \rightarrow \frac{H}{\sqrt{H_0 + \delta}}, \quad W \rightarrow (H_0 + \delta)^{-\frac{1}{4}} W (H_0 + \delta)^{-\frac{1}{4}} \quad (3)$$

where H_0 is now the non-relativistic Hamiltonian $H_0^{n.r.} = -\frac{\Delta}{2M}$ and W is the quadratic form that represents the joint weak contact (for convenience, we have chosen $M = \frac{1}{2}$).

We choose units for which $2M = 1$.

For $\delta > 0$, we can proceed as before.

One must now take the limit $\delta \rightarrow 0$.

We must prove that in the limit $\epsilon \rightarrow 0$, $\delta \rightarrow 0$ in any order no divergences occur. For this, we make use translation invariance.

For a three particle system, using translation invariance one can restrict attention to the reference frame in which the barycentre is at rest.

Placing the barycentre at the origin and using polar coordinates in momentum space one verifies that in this reference frame for a three particle system the diverging factor that occurs at zero momentum in the limit $\delta \rightarrow 0$ is cancelled by the density at the origin in polar coordinates of the three particle systems

Therefore, one can take the limit $\delta \rightarrow 0$.

We still denote by $\mathcal{K}$ this "non relativistic" Krein map.

One major difference in the non-relativistic case is the presence for each weak contact of a zero energy resonance.

Recall that for a two-particle system the presence of a zero energy resonance would prevent the use of Gamma convergence.

But for a system of three particles in mutual weak contact there is a closed chain of three zero energy resonances, i.e. an essential singularity at zero energy.

The presence of this singularity is not an obstacle for Gamma convergence. $\square$

5 The Gross-Pitaevskii equation

From now on we shall take $m = 0$ in the definition of weak contact. Weak contact is therefore associated with a zero energy resonance.

We have seen that the Krein map can be defined also in the non-relativistic case.

Proceeding as the case $m > 0$ and using barycentre and relative coordinates we obtain in $\mathcal{M}$ for three identical particles in mutual weak contact a family of self-adjoint operators with infinitely many energy resonances.

Inverting the Krein map, one has an ordered family of quadratic forms.

Gamma convergence still applies.

We summarise our findings in the non-relativistic case; they follow from Gamma convergence and explicit estimates in the space $\mathcal{M}$.

The Gross–Pitaevskii equation

$$i\partial_t\phi(x,t) = -\Delta\phi(x,t) - c\phi^3(x,t) \quad x \in \mathbb{R}^3 \quad c > 0 \quad (4)$$

describes the motion of a system of three non-relativistic bosons in mutual weak contact. The *Gross–Pitaevskii Energy Functional*

$$E(\phi) = \int [\nabla\phi(x)|^2 - c\rho^2(x); \quad \rho(x) = |\phi(x)|^2 \quad (5)$$

has an essential singularity at zero energy.

Remark 1 Recall that the Gross–Pitaevskii functional is *the variational functional* for the Gross–Pitaevskii equation, an equation for a system of three particles in mutual *weak contact*.

In this case, the functional has an essential singularity at zero energy and therefore an infinite number of solutions to the variational problem.

They are the “solitons” and prevent the system from having a Wave Operator.

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Remark 2 We will see later that the Gross–Pitaevskii functional describes *also* the Bose–Einstein condensate.

The functionals are formally the same but in the Bose–Einstein case the functional is regular at the origin and is connected with strong contact.

Remark 3 We have shown in [1] that the Newton two body system with Coulomb interaction can be regarded as semiclassical limit of weak joint three-body contact interaction.

This provides a link between the Gross–Pitaevskii equation and the (singular) Boltzmann equation for a Coulomb gas.

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In [1], we proved using Gamma convergence that the joint weak contact of three identical particles extension is limit in *strong resolvent sense* when $\epsilon \rightarrow 0$ of interactions through potentials $V^\epsilon(|x_i - x_j|) = \frac{1}{\epsilon^2} V(\frac{|x_i - x_j|}{\epsilon})$ $x_i \in \mathbb{R}^3$ where $V \in L^1(\mathbb{R}^3)$.

In Lemma 1, we proved that the same is true when $m = 0$. The two-body system has now a zero energy resonance.

As in [1], there is no operator convergence and no rate of convergence of the resolvent can be given as a function of the parameter ϵ .

Recall that resolvent convergence implies convergence of the spectrum and of the Wave Operators *but does not imply operator convergence*.

Because of the relation between a self-adjoint operators and its resolvent, sequences along which the quadratic form of the operator diverges to $+\infty$ give a contribution to the resolvent that converges to zero and have therefore no role in resolvent convergence.

As a result, there is *no estimate* on the rate of resolvent convergence when $\epsilon \rightarrow 0$.

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6 On identical particles and weak contact

We have interpreted the Gross–Pitaevskii (focusing) equation as describing a closed loop of joint contact interaction between *three wave functions*.

In this interpretation, *the Gross–Pitaevskii energy functional is quartic and the G-P equation is variational.*

One can consider now a system of arbitrary many particles in weak contact interaction.

Consider, e.g. chains of wave function in weak contact.

Chain of two particles correspond to a zero energy resonance. Also, non-self-intersection open chains correspond to zero energy resonances.

Zero energy resonances prevent compactness, and therefore, there is no solution to the variational problem that would determine a state of the system.

Since wave functions are infinitely extended weak contact *occurs everywhere in space.*

Closed loops of zero energy resonances correspond to zero energy bound states.

Closed loops of length three play a special role.

Notice that $3 \times 2 = 6$ is both the total power of ϵ^{-1} in the approximation potentials and the number of degrees of freedom of the three-particle system in the reference frame in which the barycentre is at rest.

There is an essential singularity at the bottom of the spectrum but no zero energy resonance; therefore, compactness holds and the variational problem (find the minimum of the energy) has a unique solution.

The quadratic form can be closed strongly; the resulting self-adjoint operator represents three particles in joint weak contact.

The three particles are identical and therefore the solution is invariant under permutation of the particles.

The zero energy states are the Solitons.

7 A different system. Connection with the Bose–Einstein gas

We have interpreted the Gross–Pitaevskii equation as describing a systems of three identical wave functions in mutual weak contact. The variational functional is quartic and has an essential singularity at the origin.

There is a *different system* which has the same functional as energy functional, but for this system it is regular at the origin.

It corresponds to a self-adjoint operator and describes a system of four wave functions which have three contacts *but now the contacts are strong.*

This is a system of two pairs of wave functions in which there is a strong contact between the particles in each pair and a strong contact between the barycenters of the two pairs.

Notice that weak and strong contacts are both limit of Hamiltonian with attractive potentials with support that a radius ϵ that converges to zero.

The difference is in the rate of convergence; for fixed values of ϵ , the rate of convergence is not visible and the only difference is the presence of a zero energy resonance.

Also for this configuration the number of degrees of freedom in the reference frame of the barycentre (i.e. 9) equals the "strength" of three strong contacts.

This allows the use of the Krein map and to obtain a minimal form by Gamma convergence; as before this form can be closed strongly and represents a self-adjoint operator.

This system describes the Bose–Einstein condensate.

One can represent pictorially the new system as two dipoles with a small marked spot in the barycentre.

Each dipole represents strong contact of two wave functions.

The two dipoles are in strong contact at the marked spots.

For finite values of the parameter, ϵ the dipoles and the "marked spots" are of finite width and one can estimate (e.g. by a de Finetti analysis) the probability of intersection at the marked spot of dipoles thrown at random [6,8].

The energy of this system is still described by the Gross–Pitaevskii functional

$$E(\phi) = \int |\nabla \phi(x)|^2 - c\rho^2(x); \quad \rho(x) = |\phi(x)|^2 \quad (6)$$

but now the functional has a *different* interpretation, i.e. it is the energy functional for the strong "zero range" interaction of *two density matrices*.

The Gross–Pitaevskii equation appears now as a variational equation for an energy functional and not as dynamical equation.

The energy functional differs from the G-P functional because the spectral density at bottom of the spectrum is continuous.

This difference is not visible in the analytic form of the Functional.

8 A Fermi–Dirac condensate

The Bose–Einstein condensate is a gas of two pairs of *identical* wave functions.

Each pair is made of two wave functions in strong contact, and the barycenters are in strong contact.

If one identifies each pair with a density matrix, one has a pair of density matrices in strong contact.

Fermions with opposite spin orientations can have a contact interaction, and therefore, it is possible to have a Fermi–Dirac condensate

In order to confine the system, one can impose an external potential that can be chosen of class $L^1(R^3) \cap L^2(R^3)$.

This confining potential does not alter the structure of the condensate since it can be chosen to vanish on the support of strong contact (a set of measure zero).

The confining potential can be a function that grows sufficiently fast at infinity but also to a sufficiently intense electromagnetic field if the particle is charged.

Since Gamma convergence provides an infimum of a set of quadratic forms, the same analysis we have made for a scalar potential can be repeated for the magnetic Hamiltonian H_M defined by minimal coupling.

By means of these forces, "the gas of identical pair of wave functions in strong contact" is confined (it becomes a condensate).

Recall that both weak contact interactions and strong contact interactions are limit *in strong resolvent sense* of interactions through a sequence of potentials that have support of radius decreasing to zero.

The rate of convergence is different in the two cases but for a single value of the parameter ϵ no difference between strong and weak can be made; we shall comment on this when we will discuss (briefly) Bogoliubov's theory.

The proofs we have given are variational; we have resolvent convergence, but *there is no operator convergence and no estimate of the rate of convergence*.

In conclusion, we have seen that there is a collection of clusters of *two pairs of identical wave functions*, either *Bosons or Fermions*; in the case of Fermions, they have opposite spin).

The Gross–Pitaevskii functional describes the energy of the system.

9 Bogoliubov theory

Bogoliubov theory is an attempt to describe Bose–Einstein condensation as an effective formal perturbation theory.

We have described the Bose–Einstein condensate as a collection of system of couples of wave functions; each pair interacts through strong contact (a zero range interaction), and there is a further strong contact between the barycentres of the two pairs.

Since wave functions are not localised *strong contact can occur anywhere in space*.

In Quantum Mechanics, a wave function $\phi(x)$ is not an observable, it is only a tool of the theory.

Physical significance can be given instead to correlation function $\int \bar{\phi}(x) A(x, y) \phi(y) d^3x d^3y$ with A a symmetric form.

We have attributed Bose–Einstein condensation to strong contact interaction of pairs of wave function which are in strong contact.

Bogoliubov considered a "dynamical" aspect of the theory in which connections between particles are created or destroyed by an external agent (e.g. a strong e.m. field).

We have seen that the only stable configurations for contact interactions are clusters of three particles with two strong contacts and of four particles with three strong contacts.

Therefore, changing the number of contacts can be related to changing the number of particles.

Accordingly in Bogoliubov's theory, one introduces creation and annihilation operators.

Remark Bogoliubov was led to the formulation of his theory from his work on superfluidity.

In the Ginzburg–Landau theory, the condensate is made of pairs of wave functions in weak contacts with a zero energy (Feshbach) resonance (B.C.S pairs, B.C.S stands for Bardeen, Cooper and Schrieffer) bound by a *very weak attractive force*.

Superfluidity is due to the breaking of this very weak attraction. .

The relation between this system and Bose–Einstein Condensation is usually called *B.E.C to B.C.S transition*.

But notice that in the Bose–Einstein case, the condensation is the result of *strong* contact.

Contact interactions are defined as limits of potential with potentials V_ϵ with support of radius that converges to zero with a different rate for weak and strong contact. Therefore, for finite values of ϵ no clear distinction can be made between weak and strong contact.

10 Energy spectrum in a crystal of conduction electrons which satisfy the Pauli equation

In this section, we study the spectrum of the conduction electrons in a crystal under the assumption that they satisfy the non-relativistic Pauli equation.

We prove that this spectrum is pure point and the eigenvalues scale as $\frac{c}{\log n}$ $c < 0$.

The same result would be obtained assuming the electrons satisfy the Schrödinger equation with Hamiltonian $H_0 = \frac{-\Delta}{2m}$.

The Fermi–Dirac statistics implies that not more than two electrons occupy the same state. This implies the presence, for a large enough crystal, of a "Fermi sea" of weakly bound electrons.

If the material is "doped" (it has many impurities), conductivity decreases because the number of bound states available increases and the highest occupied level is still far from the surface of the Fermi sea.

In the analysis of this problem, we use weak contact.

The "weak contact" interaction of the conduction electrons with the lattice of ions occurs at the vertex of a Bloch cell.; it is due to the Coulomb interaction with *the entire lattice of nuclei in the crystal*

Recall that Coulomb potentials decay as $V(R) = -e\frac{1}{R}$; due to this property, the interaction with the nuclei *of the entire crystal* is equivalent to weak contact at the vertices.

11 Forces on the conduction electrons

As in [1] to understand the origin of the Fermi sea consider the forces on the conduction electrons in a crystal.

Notice that here the operator that describes the free system is the non-relativistic Pauli operator.

The crystal is represented by a regular lattice in R^3 . The nuclei occupy the centre of the cells.

To simplify the analysis, we consider the case of a cubic lattice; the edges form locally a complete basis in R^3 and the lattice has Y -shaped vertices.

The borders of the cells form a graph $\mathcal{G}$ with one-dimensional edges.

As described in [1], the result holds also in the two-dimensional case provided the Bloch lattice has Y -shaped vertices.

These electrons are spin $\frac{1}{2}$ particles that satisfy the non-relativistic Pauli equation.

If one neglects the repulsion due to the other electrons, the electrons in the outer shell of an atom can be described by the Pauli equation with a Coulomb potential that is barely sufficient to bind them.

At the vertices of a Bloch cell, the wave function of the electrons in the outer shell of an atom is deformed by the Coulomb interaction *with all the nuclei in the lattice*.

Recall that the Coulomb potential scales as $\frac{1}{r}$.

By the scaling property of the Coulomb potential, the action *of the entire lattice of nuclei* on each electron is represented by a *weak contact interaction* at the vertices of the lattice. Indeed, the wave function of the electron has a sharp discontinuity at contact).

We consider negligible the forces between electrons.

There is a weak contact interaction of each conduction electron with the nuclei of the entire lattice.

12 A Krein map

Now, the free single particle is the non-relativistic operator is the Pauli operator $P = \sigma \cdot \nabla$. We have equal to $\frac{1}{2}$ the mass of the electron and the σ_k are the Pauli matrices.

The Pauli matrices σ_i , $i = 1, 2, 3$ are the generators of the $SU(2)$ group on the unit sphere

The Pauli Hamiltonian is an operator on (totally antisymmetric) functions on the direct product configuration space and of $SU(2)$; it is invariant under the joint action of the rotation group in R^3 and $SU(2)$.

Notice that for spin $\frac{1}{2}$ particles the Pauli Hamiltonian is elliptic.

Denote by W , the quadratic form that represents weak contact of the electrons with the lattice of nuclei.

Since the electrons interact separately with the entire lattice, we must introduce a Krein map.

We now proceed as in the case of the Schrödinger equation but with Hamiltonian $H_0 = \sum_{k=1}^3 -\Delta_i$.

The non-relativistic Krein map is well defined because we have a three-body problem (three electrons interact simultaneously with the nucleus).

It is convenient to choose for the Krein map the Salpeter operator $H_S \equiv \sqrt{H_P^2}$ (positive square root).

The Krein map does not act therefore on the spin. The operator H_S commutes with H_P and with the spin degrees of freedom.

Let the quadratic form W represents the interaction at the vertices.

The Krein map acts on the free three particle Pauli Hamiltonian as H_P as $H_P \rightarrow \frac{H_P}{\sqrt{H_S}}$ and on the "potential" W (due to the entire lattice of nuclei) as $W \rightarrow H_S^{-\frac{1}{4}} W H_S^{-\frac{1}{4}}$.

Also, here this map is fractioning and mixing in the space variables.

As in [1], both the free Hamiltonian and the potential are represented in $\mathcal{M}$ by self-adjoint operators; in $\mathcal{M}$, the free Hamiltonian is a (positive) pseudo-differential operator of order $\frac{1}{2}$ and the potential term is negative.

They have in $\mathcal{M}$ at the origin in configuration space the same $\frac{c}{\sqrt{|x|}}$ singularity but with opposite signs.

Therefore, [3, 4] their sum represents in $\mathcal{M}$ a one-parameter family of self-adjoint operators each with an infinite number of (spinor-valued) bound states.

The eigenvalues scale as $c \frac{1}{\sqrt{n}}$, $c < 0$.

"Inverting the map" one has a family of forms that are weakly closed, and Gamma convergence provides a self-adjoint operator.

Gamma convergence selects the infimum; this form can be closed strongly, and the resulting self-adjoint operator is the Hamiltonian of our system.

It acts separately on each of the conduction electrons.

Due to the change in operator topology, the negative part of the spectrum of this operator is still pure point and has a $\frac{c}{\log n}$, $c < 0$ distribution.

Notice that the free Pauli Hamiltonian has no mass term and corresponds to the "non relativistic" Schrödinger Hamiltonian.

There is a further weaker interaction that takes place at the centre of the edges and is due to the joint action of the nuclei that are in a section of the crystal which is perpendicular to the edge

As in the contact approximation for the Schrödinger equation, we first obtain the solution (the wave functions of the conduction electrons) on the graph and then extended it to R^3 by unique continuation.

Here, we have the same results for the Pauli equation (the Pauli equation for spin $\frac{1}{2}$ particles is elliptic), as in [1].

This is not surprisingly since the Schrödinger operator is the square of the Pauli operator

13 Reduction to the graph

Consider the barycenters of the electrons.

Remark that in the present case the contact interaction induces for each electron at a vertex of the lattice a *simultaneous* change of direction of the momentum and of spin orientation (not of the energy).

This interaction on the graph is therefore invariant under the symmetry group of the free Pauli equation.

Recall that in this case the configuration space is the space of barycenters of spin-valued functions on a graph.

We now proceed as in [1] and define *on the graph* a (generalized) Krein map $\mathcal{K}$ and a Minlos space $\mathcal{M}$.

Here, the interaction is represented by a quadratic form W that describes the change of direction of momentum *and of spin* at the vertex.

Also, here the Krein map is mixing and fractioning and one has in $\mathcal{M}$ an ordered parameter family of self-adjoint operators.

Reverting to the space of square integrable functions, one has a one parameter family of well-ordered weakly closed quadratic forms, all bounded below.

Gamma convergence holds because there are no zero energy resonances and therefore the quadratic forms belong to a compact set in a Sobolev topology.

Gamma convergence [2] selects the minimal one; the resulting form can be closed strongly [5] and defines a self-adjoint Hamiltonian.

This Hamiltonian has a family of eigenstates with eigenvalues that, due to the change in metric topology decrease now with a law $\lambda_n = -c \frac{1}{\log n}$ $c < 0$.

This is the same result that we obtained in [1] in the case of the non-relativistic Schrödinger equation (possibly with a different value of the constant c).

Remark The same analysis is valid for the magnetic Pauli operations.

Also in this case Gamma convergence selects the operators that is associated with the minimal form (i.e. the Hamiltonian defined by minimal coupling).

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14 Extension to the Bloch graph and the entire space

As remarked in [1], the extension of the solution for the barycenters on the graph can be extended, as in the case of the Schrödinger equation, to the wave function of the electrons on the entire space by unique continuation (the Pauli equation is elliptic on spinor-valued functions)

It corresponds to joining together in the middle of an edge the solution on the graph, adding the interaction at the mid-point, using periodicity and performing unique continuation inside the cell.

The continuation is a function that is continuous (as spin -valued function); it may correspond to a spin flip at the centre of the cells.

The $\frac{c}{\log n}$, $c < 0$ structure of the energy spectrum of the eigenstates makes this operation time independent (*the phases of the eigenfunction "move at the same speed"*).

The resulting eigenfunctions are in this case spinor-valued functions.

In the middle of the cells, the orientation of the spin may different then that at the boundary ($\mathbb{Z}_2$ index)

As remarked in [1] the eigenfunctions of the deepest bound states are supported near the graph.

This is confirmed by measurements performed with the aid of an electron microscope. The electron microscope "registers" only waves of moderately small wave length; it measures therefore only electron in "deep" bound states.

The measurement indicates that the density of those conduction electrons that are "more bound" is negligible outside a small neighbourhood of the graph and has a maximum at the vertex.

This is also suggested by a theoretical analysis of a two-dimensional crystals [9].

In a crystal in a stable configuration, only a small fraction of the electrons occupy the lowest energy states.

The eigenfunctions of the lesser bound electrons are more spread out in space. At the top of the point spectrum, they differ little from spinor-valued Bloch waves.

In the upper end, the spectrum is very dense (but still a point spectrum).

Since electrons satisfy the Fermi–Dirac statistics, no two of them can "occupy" the same bound state (including spin).

15 The Fermi sea

The Fermi sea is the collection of the electrons in the bound states.

It is worth recalling that in Quantum Mechanics electrons are "identical particles" that satisfy the Fermi–Dirac statistics".

No two of them can occupy the same state. The "Fermi sea" is the collection of electrons that are in a bound state.

In a large crystal, the electrons "near the surface" are weakly bound. Their wave functions are very extended and differ little from Bloch waves (magnetic Bloch waves if a magnetic field is present).

A very small external electric field is sufficient to lift to the surface of the Fermi sea the "conduction electrons" that are weakly bound and originate a current (or in the presence of a magnetic field to give magnetic polarization).

Due to the $\frac{1}{\log n}$ law of the energy levels of the bound state for large values of n the spacing is so small that they are usually considered as a *continuum* (a *band*). But in reality the spectrum is pure point and there are infinitely many gaps.

In highly "doped" crystals, there are many more different bound state and the least bound electron has still a relevant binding energy.

Therefore, conductivity decreases.

Remarrk 1 The scaling law for the energy of the bound states is the same as in the Schrödinger case. This is not surprising since the relativistic Schrödinger operator is the square of the Pauli Hamiltonian and the scaling law $\lambda_n = \frac{c}{\log n}$ is invariant under the map $\lambda_n \rightarrow \lambda_n^2$ (only the factor c changes).

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We sum up our findings in the

Proposition *In an infinite crystal, the conduction electrons have a point spectrum that follows a $\frac{c}{\log n}$ law, with $c < 0$. This is true independently of whether the electrons are described by the Pauli or the Schrödinger non-relativistic equations.*

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Remark 1 To make connection with the "macroscopic" treatment of the problem, we stress that weak contact is produced by Coulomb forces exerted on conduction electrons *by the entire (infinite) lattice of ions*.

This interaction can be interpreted *at a macroscopic scale* (e.g. at a scale in which the Bloch cell is regarded as a point) as a short-range (next-neighbour) interaction.

We recall also that Coulomb interaction is the semiclassical limit of weak contact.

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Remark 2 By energy conservation to the potential forces which with the lattice of ions acts on the conduction electrons corresponds a potential force that deforms the lattice of ions while keeping the lattice structure invariant.

The precise determination of this deformation is very difficult.

In this respect, our results are at first order in $\frac{m}{M}$ where m is the mass of the electrons and M is the mass of the nuclei.

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16 Magnetic fields

We have so far considered a crystal in the absence of magnetic field.

The Krein map can be defined also in the presence of a magnetic field; the Hamiltonian chosen by Gamma convergence corresponds still to the minimal quadratic form.

This minimal form can be closed strongly; by construction, it is the Hamiltonian that one obtains by the traditional "minimal coupling".

The Coulomb potential scales as the inverse of a length.

This allows the introduction of a "macroscopic lattice" in which the Bloch cell are regarded as vertices.

This implies a change of scale of the Pauli or Schrödinger operators, and the interaction is now a next-neighbour interaction.

In the presence of an external E.M. field, the Hamiltonian is changed (Peierls substitution) and Gamma convergence chooses the minimum of the new forms.

Notice that models of next-neighbour interaction are often introduced without noticing that they correspond to rescaling the Coulomb potential and the Laplacian (or the Pauli operator).

Under this scaling, the spectrum is still point spectrum with multiplicity two.

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