

Application of the Klein-Gordon and Bogoliubov-deGennes theories to Nickelates

Aplicación de las teorías de Klein-Gordon y de Bogoliubov-deGennes a Niquelatos

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Abstract

In the present work we show the generalities of the classical field theory (CFT), we study its extension to the quantum field theory (QFT), where as an example of numerical analysis and combination with the field theory technique, we solve a system Klein-Gordon type (KGS) in two space-time dimensions (1+1) studying its stability through the spectral parameter $\lambda(k)$, principle of convergence due to the parameters of the numerical network and the solution for the field $\phi(x;t)$, obtaining novel results. Also, we briefly study the technique of creation and destruction ladder operators from the perspective of the quantum harmonic oscillator, to define some properties and extensions to the problem in canonical quantization. Finally, we apply the topics studied to a problem of unconventional superconductivity in Nickelates compounds by solving the system of Bogoliubov-deGennes (BdG) Equations in the mean expansion of the field, obtaining the superconducting energy band.

Keywords: Quantum theory; Second quantization; Canonical quantization; Second order transformation; Bogoliubov-de Gennes; Superconductivity.

Resumen

En el presente trabajo mostramos las generalidades de la teoría clásica de campos (CFT), estudiamos su extensión a la teoría cuántica de campos (QFT), donde como ejemplo de análisis numérico y combinación con la técnica de la teoría de campos, resolveremos un sistema tipo Klein-Gordon (KGS) en dos dimensiones espacio temporales (1+1) estudiando su estabilidad mediante el parámetro espectral $\lambda(k)$, principio de convergencia debido a los parámetros de la red numérica y la solución para el campo $\phi(x;t)$, obteniendo resultados novedosos. Además, analizamos brevemente la técnica de operadores de Escalera creación y destrucción desde la perspectiva del oscilador armónico cuántico, para definir algunas propiedades y extensiones al problema en cuantización canónica. Finalmente, aplicamos los temas estudiados a un problema de superconductividad no convencional en compuestos Niquelatos solucionando el sistema de Ecuaciones de Bogoliubov-deGennes (BdG) en la expansión media del campo, obteniendo la banda energética superconductora.

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Palabras clave: Quantum theory; Second quantization; Canonical quantization; Second order transformation; Bogoliubov-deGennes; Superconductivity.

1. Introduction

In general, in classical mechanics, there are several ways to study the dynamics of particle systems [1], [2], [3], [4]. This really depends on the problem to be addressed and the possible connections with various methods to be applied. In particular, the main connection between classical mechanics and classical field theory is due to Lagrange's or Hamilton's formulations. By means of the first, a scalar function is defined, whose dependence as a functional is due to the coordinates, generalized velocities and the time $\mathcal{L}(q, \dot{q}, t)$ in addition, the canonical momentum, $p = \frac{\partial \mathcal{L}}{\partial \dot{q}}$. From variational calculus, to find a stable value, the action integral satisfies [2]:

$$\delta s = \delta \int_{t_0}^t \mathcal{L} dt = \int_{t_0}^t \left(\frac{\partial \mathcal{L}}{\partial q} \delta q + \frac{\partial \mathcal{L}}{\partial \dot{q}} \delta \dot{q} + \frac{\partial \mathcal{L}}{\partial t} \delta t \right) dt \quad (1)$$

For the problem to be well defined, the boundary conditions $\delta(q(t_0)) = \delta(q(t)) = 0$ must be found, and performing the integration we obtain:

$$\delta s = \int_{t_0}^t \left(\frac{\partial \mathcal{L}}{\partial q} \delta q - \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{q}} \right) \delta q + \frac{\partial \mathcal{L}}{\partial t} \delta t \right) dt = 0 \quad (2)$$

Taking into account the fundamental lemma of the variational calculus [5], [6], the so-called Euler Lagrange equation is obtained:

$$\frac{\partial \mathcal{L}}{\partial q} - \frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{q}} \right) + \frac{\partial \mathcal{L}}{\partial t} \delta t = 0 \quad (3)$$

With which, given a Lagrangian function, it is possible to find the equations of motion that describe the state of the system. Now, in the Lagrangian description, the dynamics of the movement is in the configuration space, where each point accounts for the state of the system at a given time. However, it is more general to study the system depending on the coordinates and generalized or conjugate moments. It is in this way that the Hamiltonian is defined, as the Legendre transform of the Lagrangian function $H = \sum_i^p \dot{q}_i p_i - \mathcal{L}$, i goes over the degrees of freedom. By varying the Hamiltonian, the Hamilton [3], [4] equations are obtained: $\dot{q} = \frac{\partial H}{\partial p}$, $\dot{p} = -\frac{\partial H}{\partial q}$. Suppose a functional A , dependent on generalized positions and moments $A(q, p)$ and take its total derivative:

$$\frac{dA}{dt} = \frac{\partial A}{\partial q} \frac{dq}{dt} + \frac{\partial A}{\partial p} \frac{dp}{dt} = \frac{\partial A}{\partial q} \dot{q} + \frac{\partial A}{\partial p} \dot{p} \quad (4)$$

Now, it is possible to define the Poisson bracket:

$$\{A, B\}_{Poisson} = \frac{\partial A}{\partial q} \frac{\partial B}{\partial p} - \frac{\partial B}{\partial p} \frac{\partial A}{\partial q} \quad (5)$$

Finally arriving at the time evolution equation, for any dynamic quantity [4], [5].

$$\frac{dA}{dt} = \{A, H\}_{Poisson} + \frac{\partial A}{\partial t} \quad (6)$$

This is the classical perspective, for the treatment of fields, with finite freedom degrees. Now, the extension that interests us to systems with infinite degrees of freedom is done as follows, initially with the relativistic notation, the index $\nu = 0; 1; 2; 3$, being $\nu = \nu_0$ temporal dependence and other indices responsible for spatial coordinates, additional Einstein notation be used. Thus, the extension of the Euler-Lagrange equation is written:

$$\partial_\nu \frac{\partial \mathcal{L}}{\partial (\partial_\nu \phi)} - \frac{\partial \mathcal{L}}{\partial \phi} = 0; \quad \nu = 0, 1, 2, 3 \quad (7)$$

With the dependence of the Lagrangian functional $\mathcal{L}(\phi, \dot{\phi}, t)$ and the field $\phi(x, t)$ and the extension to the continuum of the Hamiltonian density:

$$\begin{aligned} \mathfrak{H} &= \int d^4 x \left(\Pi(x) \dot{\phi}(x) - \mathcal{L}(\phi, \dot{\phi}) \right); \Pi \\ &= \frac{\partial}{\partial \dot{\phi}} \int \mathcal{L} d^3 x \end{aligned} \quad (8)$$

in addition, with the derivation notation $\partial_\nu^2 = \partial_t^2 - \nabla^2$, that is, given a Lagrangian as a function of a given field, the Euler-Lagrange equation is used and the equation of motion is obtained.

2. Numerical analysis of a Klein-Gordon system

As a particular example of how field theory is applied, we study the system described by the KGL in one dimension and we study its numerical bidimensional solution under that conditions where the system is unconditionally stable. Thus, we start with the Lagrangian, which describes a KGS [6], [7] type system:

$$\mathcal{L}(\phi, \dot{\phi}) = 1/2 \dot{\phi}^2 - 1/2 (\nabla \phi)^2 - 1/2 m^2 \phi^2 \quad (9)$$

where $\phi(x, t)$ represents the field. With this, the application of the Euler-Lagrange equation generates the following derivatives, proceeding with the construction of the equation of motion of the system:

$$\frac{\partial \Omega}{\partial \phi} = m^2 \phi; \quad \nabla \cdot \nabla \phi = \partial_t \frac{\partial \Omega}{\partial (\partial_v \phi)} = \ddot{\phi} \quad (10)$$

obtaining the following equation of motion:

$$\ddot{\phi} - \nabla^2 \phi + m^2 \phi = 0 \quad (11)$$

where $\ddot{\phi}$, represents the second time derivative. With this, to address the numerical solution of the KGS, we identify that it is a partial differential equation, of the hyperbolic [7], [8], [9] type. For these equations, the initial conditions are of the Gaussian type $\phi(x, 0) = e^{-x^2}$ [8], [10] and for the boundaries, the following are applied: boundary conditions $\phi(1, t) = \phi(L, t) = f(t)$ in general these conditions are Gaussian too, in addition we study a rectangular domain, whose size is L . With this, we discretize the system using the finite difference method, where we use a stencil (numerical scheme) to discretize the temporal and spatial derivative. Initially by notation, we define $\phi(x_j, t_n) = \phi_j^n$ with $0 < x < J$ and $0 < t < n$ which be used to discretize the space and time of the field $\phi(x, t)$, in each one of the points in the domain to be studied. Thus, in the central derivative scheme [8], [11], [12]:

$$\begin{aligned} \ddot{\phi} = \partial_{tt} \phi &= \frac{1}{(\Delta t)^2} (u_j^{n+1} - 2\phi_j^n + \phi_j^{n-1}); \\ \phi_{xx} &= \frac{1}{(\Delta x)^2} (u_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n) \end{aligned} \quad (12)$$

Where we consider $\nabla^2 \phi = \partial_{xx}$, just in one dimension:

$$\begin{aligned} \frac{1}{(\Delta t)^2} (u_j^{n+1} - 2\phi_j^n + \phi_j^{n-1}) \\ - \frac{1}{(\Delta x)^2} (u_{j+1}^n - 2\phi_j^n \\ + \phi_{j-1}^n) + m^2 \phi_j^n = 0 \end{aligned} \quad (13)$$

using the implicit solution scheme [8], [13], to find the propagation of the solution at points $n + 1$, given the values $n, n - 1, \dots$, i.e ϕ_j^{n+1} given the interior points of the lattice, we obtain:

$$\begin{aligned} \phi_j^{n+1} = (2(1 - v^2) - m^2 \Delta t^2) \phi_j^n + \\ v^2 (\phi_{j+1}^n + \phi_{j-1}^n) - \phi_j^{n-1} \end{aligned} \quad (14)$$

where $v = (\Delta t / \Delta x)^2$. This stencil accounts for the temporal evolution of the solution of the field ϕ_j^n . However, at this point it is not known whether the system is stable, unstable or chaotic. The standard method is to perform the amplifier calculation of the number system

[13], [15]. Thus, we consider Newmann's method as the basis of this analysis. Suppose that the solution of the system is separable, using the Fourier method [8], [14], [15].

$$\phi_j^n = \lambda^n e^{ikJ\Delta x} \quad (15)$$

where k , is a constant and Δx the size of the network. We define $\phi_j^{n+1} = \lambda \lambda^n e^{iJk\Delta x}$, $\phi_{j+1}^n = \lambda^n e^{iJk\Delta x} e^{ik\Delta x}$, $\phi_{j-1}^n = \lambda^n e^{iJk\Delta x} e^{-ik\Delta x}$, $\phi_j^{n-1} = \lambda^n \lambda^{-1} e^{-iJk\Delta x}$ and for simplification in the notation we call a $(2(1 - v^2) - m^2 \Delta t^2) = \tilde{m}^2$. We get the algebraic equation for the amplifier: $\lambda^2(k) - \lambda(k)(\tilde{m}^2 + 2v \cos(k\Delta x)) + 1 = 0$. Since the roots are complex for every value of k ($|\lambda(k)| < 1$), in general the scheme is conditionally stable, if $v > 1$. Where for simplicity we take $a = \tilde{m}^2 + 2v \cos(k\Delta x)$ and the possible values for $\lambda(k)$ are found by solving the equation: $\lambda_1 = \frac{1}{2}(a - \sqrt{a^2 - 4})$, $\lambda_2 = \frac{1}{2}(sqrt{a^2 - 4} + a)$ with $a = \tilde{m}^2 + 2v \cos(k\Delta x)$, these values of the amplification factor, realize that the system is conditionally stable, this conditioning depends on geometric parameters of the network or numerical mesh.

To analyze the KGS problem, we initially consider the coefficient m^2 and find the non negative values as follows: $(2(1 - v^2) - m^2 \Delta t^2) > 0$, and $\Delta t > \sqrt{\frac{2(1-v^2)}{m^2}}$.

This is the mesh size in the temporal direction, which depends on the eigenvalues of the studied system, this indicates the values that must be taken into account for the solution of the system. Now with the information of the system, the size of the network, initial conditions and boundary conditions, for $\phi(x, t)$ we proceed to present the numerical solution of the KGS type system. So, we take as initial condition $\phi(x, 0) = e^{-(x-0.2)^2}$ and boundary conditions $\phi(1, t) = \phi(L, t) = e^{-(x_i-t-0.2)^2}$ with $x_i = 1, L$. We present in Figure 1 the solution for $\phi(x, t)$ and its temporal evolution for different times t , where the constants were taken as $m = 1$, $dx = 0;02$, $dt = 0;1$, $v = 0;2$ and total points in time $Nt = 100$. We observe the agreement of the solution for the field $\phi(x, t)$, with respect to other techniques used for its solution [16], [17].

We observe that the coincidence between the method used and other techniques, which involve greater refinement of the network and extensions, is almost complete. Additionally, in Figure 2, we present the projection of the solution for a fixed time $t = 0;01$, which is consistent with the hyperbolic behavior of the KGS.

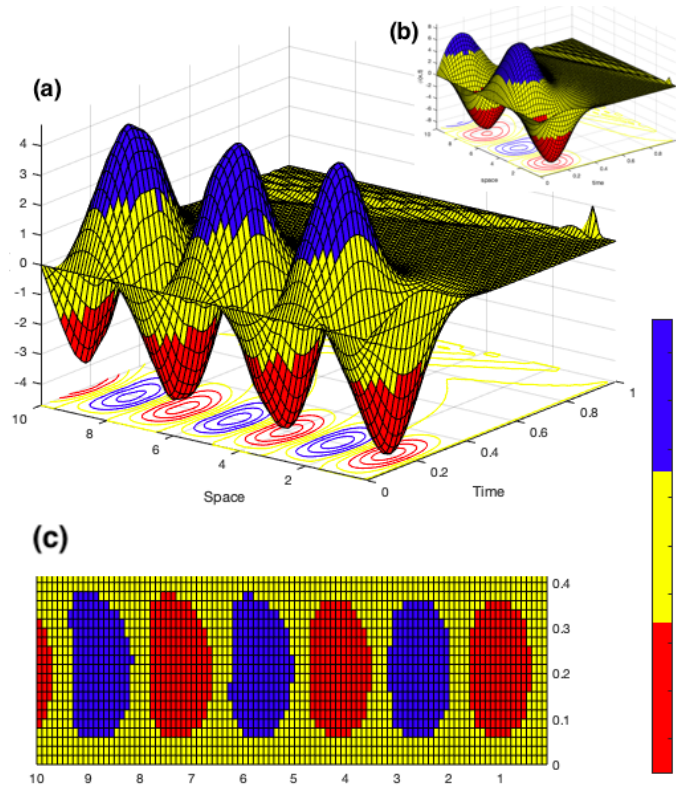


Figure 1. (a) Numerical solution of KGS for the field $\phi(x, t)$ with initial condition $\phi(x, 0) = e^{-(x-0.2)^2}$ and boundary conditions $\phi(1, t) = \phi(L, t) = e^{-(x_i-t-0.2)^2}$ with $x_i = 1, L$ according to its border. (b) Same solution, with difference in size in the domain and (c) projection for of the solution.

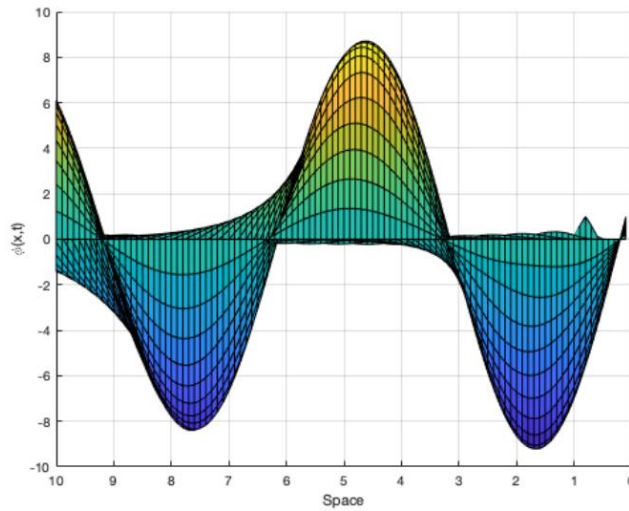


Figure 2. Projection of the numerical solution of KGS for the field $\phi(x, t)$, with initial condition $\phi(x, 0) = e^{-(x-0.2)^2}$ and boundary conditions $\phi(1, t) = \phi(L, t) = e^{-(x_i-t-0.2)^2}$, with $x_i = 1, L$ according to its boundary.

Additionally $\lim_{t \rightarrow \infty} \phi(x, t) = 0$ which defines the asymptotic behavior of the complex scalar field [14]. As an aside, we reaffirm the importance of the sample size in the time direction Δt , since this condition is highly unstable, i.e for values close to said step for time, the

system becomes unstable and possibly chaotic, this study for the size and for the spectral factor, have not been studied before [18], therefore, this is a novel result in this work.

Finally, in the **Figure 3**, we present the difference between $|\phi_{j+1}^{n+1} - \phi_j^n|$, for different iterations, we observe that in general for the first iterations the error is relatively large and then begins a marked decrease for values greater than 14, having a first minimum for the iteration 23 and then an increase in this difference for values $39 < i < 49$, followed by an increase, this behavior is common for conditionally stable systems, where this maximum oscillatory difference.

3. Application of quantum field theory, Bogoliubov-deGennes equations and mean field

One of the most fruitful theories since its appearance for the study of quantum field theory in systems with second order phase transformation; i.e superconductors, it was the BCS (Bardeen-Cooper-Schrieffer) theory, this was the first theory to study the phenomenon of superconductivity from the microscopic view of the phenomenon and to be the first to correctly describe the superconducting gap in function of temperature [19], [20]. However, the extensions of said theory have been widely applied in different contexts; such as the expressions of BdG, Migdal-Eliasberg and extensions to phenomenological descriptions, such as those due to GinzburgLandau (TDGL) and Gross-Pitaevskii (BEC). To do this, we start from the Fourier transform between the creation and destruction operators, from the real space to the space of moments.

$$\begin{aligned}\hat{a}(r\sigma) &= \sum_{k,\sigma} e^{ikr} \hat{a}_{k,\sigma}; \hat{a}^\dagger(r\sigma) \\ &= \sum_{k,\sigma} e^{-ikr} \hat{a}_{k,\sigma}^\dagger\end{aligned}$$

With \hat{a} (\hat{a}^\dagger) destroys (creates) a particle at position i , additional, σ , represents the spin operator (up $\uparrow \sigma$, down $\downarrow \sigma'$), in conjunction with the normalization rule already used $\int u^*(x)u(x)d^3x = 1$ we proceed to the construction of the Hamiltonian density, with $\hat{H} = \frac{\hat{p}^2}{2m} + \hat{U}$.

$$\begin{aligned}\mathfrak{H} &= \int d^3r \hat{a}^\dagger \hat{H} \hat{a} \\ &= \int d^3r \sum_{k,\sigma} e^{-ikr} \hat{a}_{k,\sigma}^\dagger \left(\frac{\hat{p}^2}{2m} + \hat{U} \right) e^{ikr} \hat{a}_{k,\sigma}\end{aligned}\quad (16)$$

and

$$\begin{aligned}\mathfrak{H} &= \sum_{k,\sigma} \hat{a}_{k,\sigma}^\dagger \left(\frac{\hat{p}^2}{2m} + \hat{U} \right) \hat{a}_{k,\sigma} \int d^3r e^{-ikr} e^{ikr} \\ &= \sum_{k,\sigma} \hat{a}_{k,\sigma}^\dagger \left(\frac{\hat{p}^2}{2m} + \hat{U} \right) \hat{a}_{k,\sigma}\end{aligned}\quad (17)$$

Which is the so-called free Hamiltonian, where the potential \hat{U} , represents impurities or deformations in the crystal lattice of the system used. The second part of the Hamiltonian, was included by the authors of BCS, by means of this addition the interaction behavior of the electrons due to the possible oscillations of the network is explained, these paired electrons were called Cooper pairs.

$$\mathfrak{H}_2 = -\frac{V}{2} \sum_{k,k',\sigma,\sigma'} \hat{a}_{k,\sigma}^\dagger \hat{a}_{k',\sigma'}^\dagger \hat{a}_{k',\sigma} \hat{a}_{k,\sigma}\quad (18)$$

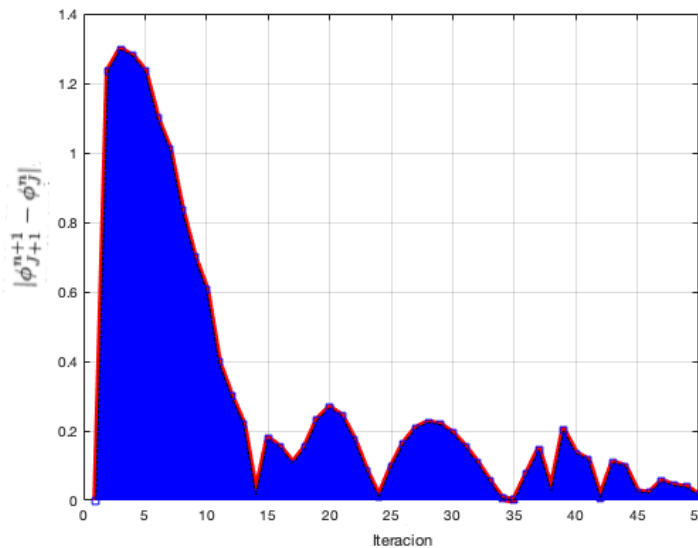


Figure 3. Oscillatory difference for $|\phi_{j+1}^{n+1} - \phi_j^n|$, as a function of iteration.

Whereupon the BCS Hamiltonian is completely rewritten as follows:

$$\begin{aligned} \mathfrak{H}_2 &= \sum_{k,\sigma} \hat{a}_{k,\sigma}^\dagger \hat{H} \hat{a}_{k,\sigma} \\ &- \frac{V}{2} \sum_{k,k',\sigma,\sigma'} \hat{a}_{k,\sigma}^\dagger \hat{a}_{k',\sigma'}^\dagger \hat{a}_{k',\sigma} \hat{a}_{k,\sigma} \end{aligned} \quad (19)$$

In the initial BCS theory, the repulsion potential between electrons is defined as negative and constant and is present in the repulsion term as V . With this, the solution of the eigenstates of the Hamiltonian BCS accounts for the variation of the coupling between the free electrons, i.e. there is a frequency that describes the union of this coupling between electrons, this energy value is called superconducting Gap. The idea in the BdG theory is to carry out the mean field expansion of the BCS Hamiltonian generating the spatial study of the Gap, thus:

$$\begin{aligned} \mathfrak{H}_{BdG} &= \langle \langle \mathfrak{H}_{BCS} \rangle \rangle = \langle \langle \sum_{k,\sigma} \hat{a}_{k,\sigma}^\dagger \hat{H} \hat{a}_{k,\sigma} \rangle \rangle - \\ &\langle \langle \frac{V}{2} \sum_{k,k',\sigma,\sigma'} \hat{a}_{k,\sigma}^\dagger \hat{a}_{k',\sigma'}^\dagger \hat{a}_{k',\sigma} \hat{a}_{k,\sigma} \rangle \rangle \end{aligned} \quad (20)$$

The first term accounts for the energy of the system, the second term describes the interaction between the electrons, we study this mean value using Wick's theorem [7].

$$\begin{aligned} -\langle \langle \frac{V}{2} \sum_{k,k',\sigma,\sigma'} \hat{a}_{k,\sigma}^\dagger \hat{a}_{k',\sigma'}^\dagger \hat{a}_{k',\sigma} \hat{a}_{k,\sigma} \rangle \rangle &= \\ -\langle \langle \frac{V}{2} \sum_{k,k',\sigma,\sigma'} [\langle \hat{a}_{k,\sigma}^\dagger \hat{a}_{k',\sigma'}^\dagger \rangle \hat{a}_{k',\sigma} \hat{a}_{k,\sigma} + \hat{a}_{k,\sigma}^\dagger \hat{a}_{k',\sigma}^\dagger \langle \hat{a}_{k',\sigma} \hat{a}_{k,\sigma} \rangle + \langle \hat{a}_{k,\sigma}^\dagger \hat{a}_{k',\sigma}^\dagger \rangle \langle \hat{a}_{k',\sigma} \hat{a}_{k,\sigma} \rangle] \rangle \end{aligned}$$

Where the gap is defined as $\Delta(r) = -V/2 \langle \langle \hat{a}_{k',\sigma'} \hat{a}_{k,\sigma} \rangle \rangle$ and $\Delta^* = -V/2 \langle \langle \hat{a}_{k,\sigma}^\dagger \hat{a}_{k',\sigma'}^\dagger \rangle \rangle$, with which equating in the previous expression, we obtain the first form of the Hamiltonian BdG:

$$\begin{aligned} \mathfrak{H}_{BdG} &= \sum_{k,\sigma} \hat{a}_{k,\sigma}^\dagger \hat{H} \hat{a}_{k,\sigma} \\ &+ \sum_{k,k',\sigma,\sigma'} [\Delta(r) \hat{a}_{k,\sigma}^\dagger \hat{a}_{k',\sigma'}^\dagger + \Delta^*(r) \hat{a}_{k',\sigma'} \hat{a}_{k,\sigma} + |\Delta(r)|^2] \end{aligned} \quad (21)$$

Where it is observed that there is a spatial dependence of the Gap $\Delta(r)$. Now, with the use of canonical quantization, for fermions (see equation 24), where we observe that the BdG Hamiltonian can be written as a

quadratic version in the base of the occupations, so we define it as the effective Hamiltonian:

$$\mathfrak{H}_{\text{eff}} = E_g + \sum_{n,\sigma} E_n \Gamma_{n,\sigma}^\dagger \Gamma_{n,\sigma} \quad (22)$$

$$\{\Gamma_{n,\sigma}, \Gamma_{n',\sigma'}^\dagger\} = \delta_{n,n'} \delta_{\sigma,\sigma'} \quad (23)$$

$$\{\Gamma_{n,\sigma}^\dagger, \Gamma_{n',\sigma'}^\dagger\} = \{\Gamma_{n,\sigma}, \Gamma_{n',\sigma'}\} = 0 \quad (24)$$

With which, we proceed to develop the properties of the anti-commutators between the effective Hamiltonian and the operators $\Gamma_{n,\sigma}$ and $\Gamma_{n,\sigma}^\dagger$:

$$\begin{aligned} \{\hat{H}_{\text{eff}}, \Gamma_{n,\sigma}\} &= \{E_g + \sum_{n,\sigma} E_n \Gamma_{n,\sigma}^\dagger \Gamma_{n,\sigma}, \Gamma_{n,\sigma}\} = \\ &\{E_g, \Gamma_{n,\sigma}\} + \left\{ \sum_{n,\sigma} E_n \Gamma_{n,\sigma}^\dagger \Gamma_{n,\sigma}, \Gamma_{n,\sigma} \right\} = \\ &\sum_{n,\sigma} E_n \{\Gamma_{n,\sigma}^\dagger \Gamma_{n,\sigma}, \Gamma_{n,\sigma}\} = \\ &\sum_{n,\sigma} E_n (\Gamma_{n,\sigma}^\dagger \{\Gamma_{n,\sigma}, \Gamma_{n,\sigma}\} - \Gamma_{n,\sigma} \{\Gamma_{n,\sigma}, \Gamma_{n,\sigma}^\dagger\}) = \\ &\{\hat{H}_{\text{eff}}, \Gamma_{n,\sigma}\} = -E_n \Gamma_{n,\sigma} \end{aligned}$$

For the construction of the BdG equation system, we proceed to calculate the anti-commutation relation between the Hamiltonian of the equation 28 with the operators $\hat{a}_{k,\sigma}$ and $\hat{a}_{k,\sigma}^\dagger$:

$$\begin{aligned} \{\hat{a}_{k,\sigma}, \mathfrak{H}_{BdG}\} &= \{\hat{a}_{k,\sigma}, \sum_{k,k',\sigma,\sigma'} [\Delta(r) \hat{a}_{k,\sigma}^\dagger \hat{a}_{k',\sigma'}^\dagger + \Delta^*(r) \hat{a}_{k',\sigma'} \hat{a}_{k,\sigma} + |\Delta(r)|^2] + \sum_{k,k',\sigma,\sigma'} \{\hat{a}_{k,\sigma}, \Delta(r) \hat{a}_{k,\sigma}^\dagger \hat{a}_{k',\sigma'}^\dagger + \{\hat{a}_{k,\sigma}, \Delta^*(r) \hat{a}_{k',\sigma'} \hat{a}_{k,\sigma}\} + \{\hat{a}_{k,\sigma}, |\Delta(r)|^2\} \} \end{aligned}$$

applying the anti-commutation rules, we settle on the last three terms of this expression, where $\Delta(r)$ and Δ^* have no direct dependency on k or σ :

$$\begin{aligned} \sum_{k,k',\sigma,\sigma'} \Delta(r) \{\hat{a}_{k,\sigma}, \hat{a}_{k,\sigma}^\dagger \hat{a}_{k',\sigma'}^\dagger\} + \Delta^*(r) \{\hat{a}_{k,\sigma}, \hat{a}_{k',\sigma'} \hat{a}_{k,\sigma}\} + \{\hat{a}_{k,\sigma}, |\Delta(r)|^2\} &= \\ \sum_{k,k',\sigma,\sigma'} \Delta(r) \{\hat{a}_{k,\sigma}, \hat{a}_{k,\sigma}^\dagger \hat{a}_{k',\sigma'}^\dagger\} &= \\ \{\hat{a}_{k,\sigma}, \mathfrak{H}_{BdG}\} = + \sum_{k,k',\sigma,\sigma'} \Delta(r) \hat{a}_{k',\sigma'}^\dagger & \end{aligned}$$

where $\{\hat{a}_{k,\sigma}, \hat{a}_{k',\sigma'} \hat{a}_{k,\sigma}\} = \{\hat{a}_{k,\sigma}, |\Delta(r)|^2\} = 0$. Thus, following the same process, we obtain:

$$\{\hat{a}_{k,\sigma}^\dagger, \mathfrak{H}_{BdG}\} = \sum_{k,k',\sigma,\sigma'} -\Delta(r) \hat{a}_{k',\sigma'}^\dagger$$

Finally, through the Bogoliubov transformation:

$$\begin{aligned}\hat{a}^\dagger(r, \sigma) &= \sum_n u_n^* \Gamma_{n, \sigma}^\dagger + v_n \Gamma_{n, \sigma} \\ \hat{a}(r, \sigma) &= \sum_n v_n^* \Gamma_{n, \sigma}^\dagger + u_n \Gamma_{n, \sigma}\end{aligned}\quad (25)$$

and combining the results of the anti-commutators:

$$\begin{aligned}\{\hat{a}_{k, n}, \mathfrak{H}_{\text{BdG}}\} &= \sum_{k, k', \sigma, \sigma'} \hat{H} \hat{a}_{k, \sigma} + \Delta(r) \hat{a}_{k', \sigma}^\dagger \\ \{\hat{a}_{k, n}^\dagger, \mathfrak{H}_{\text{BdG}}\} &= \sum_{k, k', \sigma, \sigma'} \hat{H} \hat{a}_{k, \sigma} - \Delta(r)^* \hat{a}_{k', \sigma}^\dagger\end{aligned}\quad (26)$$

and equating the Bogoliubov transformation:

$$\begin{bmatrix} u_n \\ v_n \end{bmatrix} E_n = \begin{bmatrix} \hat{H} & \Delta(r) \\ \Delta^*(r) & -\hat{H}^* \end{bmatrix} \begin{bmatrix} u_n \\ v_n \end{bmatrix}\quad (27)$$

What is the set of equations of BdG. Now, all that remains is to establish the self-consistency relationship for the system. Again from the Hamiltonian in the mean field and we perform the variation:

$$\begin{aligned}\delta \langle \mathfrak{H}_{\text{BdG}} \rangle &= \delta \langle \sum_{k, \sigma} \hat{a}_{k, \sigma}^\dagger \hat{H} \hat{a}_{k, \sigma} \\ &> + \sum_{k, k', \sigma, \sigma'} [\Delta(r) \delta \langle \hat{a}_{k, \sigma}^\dagger \hat{a}_{k', \sigma}^\dagger \\ &> + \Delta^*(r) \delta \langle \hat{a}_{k', \sigma} \hat{a}_{k, \sigma} \rangle]\end{aligned}$$

With $\delta |\Delta(r)|^2 = 0$ and performing the same process for the BCS Hamiltonian in mean field:

$$\begin{aligned}\delta \langle \mathfrak{H}_{\text{BdG}} \rangle &= \delta \langle \sum_{k, \sigma} \hat{a}_{k, \sigma}^\dagger \hat{H} \hat{a}_{k, \sigma} \\ &> - \\ &= -\frac{V}{2} \sum_{k, k', \sigma, \sigma'} [\delta \langle \hat{a}_{k, \sigma}^\dagger \hat{a}_{k', \sigma}^\dagger \\ &> \hat{a}_{k', \sigma} \hat{a}_{k, \sigma} + \hat{a}_{k, \sigma}^\dagger \hat{a}_{k', \sigma}^\dagger \\ &< \hat{a}_{k', \sigma} \hat{a}_{k, \sigma} \rangle + \delta \langle \hat{a}_{k, \sigma}^\dagger \hat{a}_{k', \sigma}^\dagger \\ &> \langle \hat{a}_{k', \sigma} \hat{a}_{k, \sigma} \rangle]\end{aligned}$$

4. Numerical Solution of the Klein-Gordon and Bogoliubov-deGennes Equations for Nickels

We present the numerical solution for a system of extensive current importance, which are those systems that present coexistence of superconductivity and ferromagnetism, the most innovative are those materials known as nickelates [21], [22], [23], [24], [25], [26], [27], [28], [29], and superconductors [30], [31], [32]. With this, in Figure 4 we present the crystalline structure used for the study using the BdG formalism.

In addition, in Figure 5, we present a side view of the $RNiO_2$, compound, in order to present the locations of the atoms and the potentials that be taken into account for the construction of the BdG Hamiltonian.

Given these results of quantum field theory, applied to condensed matter, specifically to second order phase transition systems, we proceed to perform a multi-band extension of the BdG system, by choosing the following Hamiltonian:

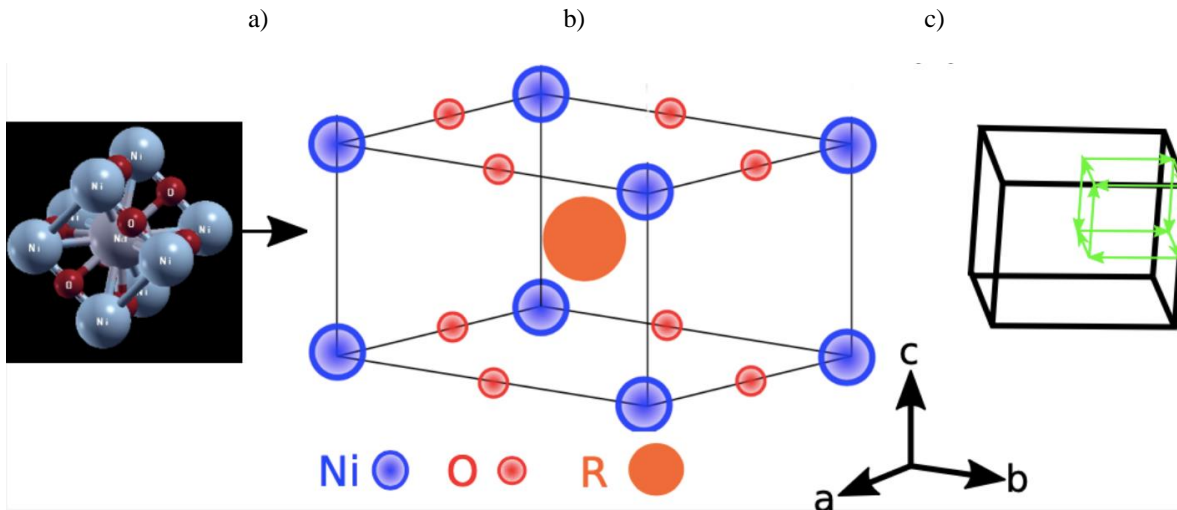


Figure 4. System studied using the BdG model $RNiO_2$, where R is Nd , Yb or Pr , (b) two layers of the compound $RNiO_2$, where Ni atoms are the blue circles, O the red circles and R are the orange circles. (c) First Brillouin zone of the $RNiO_2$ system.

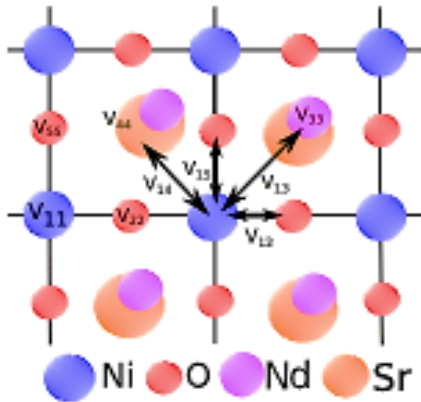


Figure 5. Representación esquemática de los átomos en una sola capa. Los átomos azules son $Ni-d_{x^2+y^2}$, los rojos son $O-2p$, los rosados son $Nd-d_{x^2+y^2}$ y $Sr-s$.

$$\begin{aligned}
 H &= \sum_{\chi\chi',p\sigma} \epsilon_{\chi,\sigma}(p) a_{\chi,p,\sigma}^\dagger a_{\chi',p,\sigma} \\
 &- \sum_{\chi\chi',p,q} V_{\chi\chi'}(p,q) a_{\chi,p}^\dagger a_{\chi',-p} a_{\chi',-q} a_{\chi,q} \\
 &+ \sum_{i,\sigma} (e_{i\sigma}^0 - \mu) n_{i\sigma}^\chi,
 \end{aligned} \quad (28)$$

We treat this Hamiltonian in mean field approximation, with inter-orbital interaction only with the first few neighboring orbitals:

$$\begin{aligned}
 \Delta_{\chi,p} &= \Delta_\chi f_{\chi,p} \\
 &= \sum_{\beta} \sum_q V_{\chi\chi'}(0) f_{\chi,p} f_{\beta,q} \frac{\Delta_{\chi'} f_{\beta,q}}{2E_{\beta,q}} \tanh\left(\frac{\beta}{2} E_{\chi',q}\right)
 \end{aligned} \quad (29)$$

Now, in the Table 1 we can define the different types of pairings between the orbitals, which account for the possible types of interaction between them, for each of the atoms presented in Table 1 and Figure 5, additional, we proceed to take a limit for a large number of particles in the system, as follows in spherical coordinates:

$$\begin{aligned}
 \sum_p &\rightarrow \int d^2p (2\pi)^2 = \int \frac{pdpd\phi d\theta}{(2\pi)^2} \rightarrow \\
 &p_\alpha(0) \int_0^{\omega_D} d\epsilon_{\alpha,p} \int_0^{2\pi} \frac{d\phi}{2\pi} \int_0^{2\pi} d\theta,
 \end{aligned} \quad (30)$$

Thus, with the construction of the Hamiltonian, a tridiagonal system by blocks is obtained in the Hamiltonian Matrix. In general, the method used for this solution is by factoring LU [9]. By implementing diagonalization, the eigenvalues and eigenfunctions for

said Hamiltonian are found. Thus, we make the graph of the superconducting gap (eigenvalues), for different values of temperature. These results are presented in the Figure 6, for different values of the mating orbital function as a function of temperature, results that coincide with the experimental results [33], [34], [35], [36], [37].

Tabla 1. Nearby neighbor mating functions in the system studied via BdG

Appearance type	Value
Singlete función tipo s	$f_p \rightarrow f_{\theta,\phi} = 1$
P-type triplet	$f_p \rightarrow f_{\theta,\phi} = \sqrt{\frac{3}{2}} \sin(\theta)$
Type $d_{x^2-y^2}$	$f_p \rightarrow f_{\theta,\phi} = \cos(2\phi)$

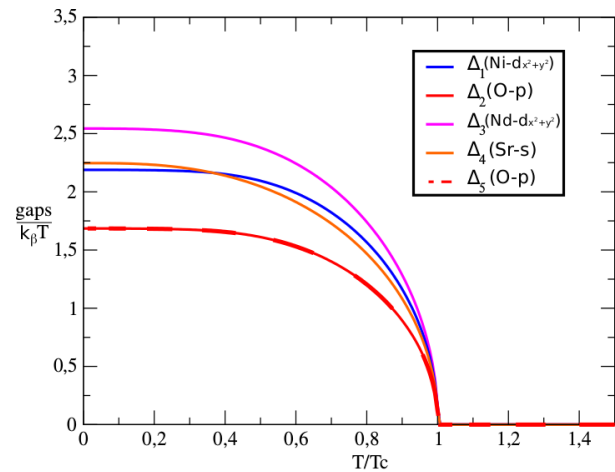


Figure 6. Gaps $k_{\beta} T_c$ as a function of T/T_c for different types of inter-orbital interaction between potentials $V_{\chi\chi'}$. The inter-orbital potential is $V_{\chi\chi} = 0$.

5. Conclusions

In this work we approach the CFT, we define its generalities and the way of proceeding from this theory, in the different physical systems. Additionally, we study the extension for QFT and as a special case we address a particular case, which is KGS, this was approached from the numerical perspective, finding novel solutions of the field $\psi(x,t)$, the amplification $(\lambda(k))$, the dependence of the stability in the solution with respect to the size of the network and the dependence of the difference $|\phi_{j+1}^n - \phi_j^n|$, with iteration. Thus we show the oscillation of the minimum convergences depending on the iteration. Then, we extend these operators to quantum field theory, through the canonical quantization of Bosons and Fermions. In addition, we expand from the BCS Hamiltonian to the BdG extension, accounting for all its

main properties, which describe superconducting systems, in a second-order transition in quantum systems. Finally, we apply the BdG formulation to an extensively studied current problem, obtaining numerical results that coincide with experimental results.

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Author Contributions

C. Aguirre: Conceptualization, Data curation, Investigation, Writing original draft, Writing - review and editing. J. Faundez: Investigation, Validation, Writing - review and editing. J. Barba-Ortega: Investigation, Validation, Writing - review and editing. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest

The authors declare no conflict of interest.

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