An effective field theory model for one-dimensional CH chains: effects at finite chemical potential, temperature and external Zeeman magnetic field

Heron Caldas

Departamento de Ciências Naturais, Universidade Federal de São João del Rei, 36301-160, São João del Rei, MG, Brazil
E-mail: hcaldas@ufsj.edu.br

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Abstract. In this work we use an effective field theory model to investigate doped (CH)$_x$ chains under the influence of an external constant Zeeman magnetic field $B_0$, at zero and finite temperature, in the mean-field approximation and beyond. We consider both homogeneous and inhomogeneous $\Delta(x)$ condensates and calculate the Pauli magnetization and the magnetic susceptibility of these chains in various situations for the temperature and chemical potentials. We also briefly discuss the possibility of using these materials as partially polarized 1D organic conductors.

Keywords: quantum wires (theory), phase diagrams (theory), electrical and magnetic phenomena (theory)
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1. Introduction

In the last few years graphene has attracted the attention of both theoretical and experimental communities due to the interesting features that this two-dimensional system presents. The electrons of this material are Dirac-like, with linear dispersion relations near the K points. Monolayer graphene can be cut into strips to construct one-dimensional (1D) graphene wires, which have been studied in various recent works [1,2]. In [3], an effective field theory has been used to investigate the low energy quantum electrodynamics of Dirac electrons in an undoped graphene wire.

Another organic material which presents similarities with a graphene wire is a CH chain, which has also attracted attention for more than three decades due to the unexpected and fascinating discovery that doped trans-polyacetylene (TPA), a 1D polymer, behaves as a metal, exhibiting the electrical conductivity of some metals, like copper [4]. Since then, several promising properties, such as electronic, optical and magnetic ones, have been shown for conjugated polymers, which indicates the possibility of the application these materials in the semiconductor nanotechnology [5,6].

Polyacetylene is a linear chain of CH groups which can have two forms, trans and cis. The trans form is more stable and, in the absence of doping, has a doubly degenerate ground state. The trans-(CH)$_x$ form has one $\pi$-electron per site, and would be a metal in the tight-binding approximation. However, spontaneous Peierls dimerization (i.e., the interaction of the electrons with the lattice) turns TPA into an insulator. After critical doping, the conductivity of TPA is greatly increased, reaching metal-like properties [7]. Experiments show that the observed non-metal to metal first-order transition in polyacetylene happens when the dopant concentration $y$, defined as the number of doped electrons per 100 carbon atoms, is increased up to a critical value $y_c \approx 6$ [8]. Recent calculations show that thermal effects have a weak effect on $y_c$ [9].

The electron–phonon interaction in CH is successfully described by the Su–Schrieffer–Heeger (SSH) Hamiltonian [10], whose continuum version is known as the Takayama–Lin–Liu–Maki (TLM) model [11]. The TLM model is a relativistic field theory with two-flavor Dirac fermions. We shall use the Gross–Neveu (GN) model [12] in 1 + 1 dimensions since its Lagrangian is equivalent to that of the TLM model [13,14]. The GN model is a well-known 1D theory with four-fermion interactions. The choice of employing an effective quantum field theory model (QFTM) in the investigation that we do in the present work is basically motivated by the analytical and simple solutions that the GN model provides, as we will see below. Besides, one of the most important features of the GN model which enables its use as an effective theory for describing materials that undergo transitions from non-metallic to metallic phases, such as the polymers that we are considering, is that it is asymptotically free, just like QCD. This means that the fermions become noninteracting at high enough densities and are not able to support the condensate that they formed to break chiral symmetry at zero or very low densities. Therefore, since the theory displays a phase transition at a certain fermion density or at the corresponding value of the chemical potential, the use of the GN model is highly appropriate in this context. In other words, or in the field theory language, the discrete chiral symmetry is spontaneously broken in the GN model and there is a dynamical generation of a mass (gap) for the electrons. A global chemical potential $\mu$ is introduced in the theory to represent the extra electrons that are inserted in the system by the doping process. At a critical chemical potential
\[ \mu_c = \Delta_0 / \sqrt{2} \] [15], where \( \Delta_0 \approx 0.7 \text{ eV for } \text{trans-(CH)}_x \) is the constant band-gap, the GN model undergoes a first-order phase transition to a symmetry restored (zero-gap) phase, agreeing with the experimentally observed non-metal to metal first-order transition in TPA [8]. Although sometimes we shall refer to TPA throughout the paper (due to the large amount of data available for it), the main results are applicable to any 1D chain with the same structure as (CH)_x.

The critical doping concentration can be related to the critical chemical potential as

\[ y_c = \left( \frac{N}{\pi \hbar v_F} \right) a \mu_c \] [16], where \( N = 2 \) can be regarded as an internal number (spin) of fermion flavors, \( h \) is Planck’s constant divided by \( 2\pi \), \( v_F = k_F \hbar / m \) is the Fermi velocity, \( k_F \) is the Fermi wavenumber, \( m = \hbar^2 / 2t_0 a^2 \), and \( a \) (\( \approx 1.22 \text{ Å for } \text{trans-(CH)}_x \)) is the lattice (equilibrium) spacing between the \( x \) coordinates of successive CH radicals in the undimerized structure, and \( t_0 \approx 3 \text{ eV for } \text{trans-(CH)}_x \) [7] is the intercarbon transfer integral for \( \pi \) electrons, known as the ‘hopping parameter’. In [16] the GN model has been used in the large \( N \) (mean-field) approximation as an effective model for describing the non-metal to metal phase transition in TPA, and they found a very good agreement with the experimentally measured \( y_c \) (\( \approx 6\% \)).

In this work we use the GN model as a QFTM for doped (CH)_x chains to investigate the consequences of \( B_0 \) applied parallel to these ‘wires’ at zero and finite temperature (\( T \)). We show that the actuation of \( B_0 \) produces an imbalance between the chemical potentials (and consequently in the densities) of the spin-up (\( \uparrow \)) and spin-down (\( \downarrow \)) conduction electrons inserted in the system. Depending on the level of imbalance between the chemical potentials of the two fermionic species involved, the (CH)_x chain can be in a non-condensed (zero-gap) partially polarized state or can be turned into a fully polarized state with a small but non-zero gap [17]. It is shown that in \text{trans-(CH)}_x with low imbalance (with respect to \( \mu_c \)), at zero \( T \), the system acquires a partial spin polarization. With strong imbalance there is total absence of electrons from one of the two possible spin orientations (\( \uparrow \) or \( \downarrow \)), meaning that the system is now fully polarized [17]. We expect this to perhaps have observable consequences in the magnetic properties of doped (CH)_x or other conducting polymers. In the investigation of spin-polarized phases and the magnetic properties of 1D \text{cis} - polyacetylene, one has to consider the massive Gross–Neveu model [18], as we shall do here.

It is important to notice that the study of the effects of an external constant Zeeman magnetic field \( B_0 \) applied to a physical system is relevant in many physical situations, as in the investigation of metal–insulator transitions [19] and magnetization [20] in 2D electron systems.

The paper is organized as follows. In section 2 we introduce the discrete and continuum model Hamiltonians and the model Lagrangian describing (CH)_x chains. In section 3 the temperature dependent renormalized effective potential is obtained in the mean-field approximation and beyond. In this section we obtain an analytical expression for the effective potential at high temperature, as well as the chemical potential dependent gap equation and the critical temperature at which the gap vanishes. Besides, the tricritical points of the second-order transition line of the gap parameter are explicitly calculated by considering both homogeneous and inhomogeneous gap parameters. The temperature dependent magnetic properties of (CH)_x chains are also obtained in this section. For completeness we study in section 4 the massive Gross–Neveu model which is appropriate for describing \text{cis} - polycetylene. In section 5 we show a summary of the main results and, finally, we present the conclusions in section 6.
2. The discrete and continuum models

2.1. The model Hamiltonians

2.1.1. The SSH discrete model Hamiltonian. The tight-binding SSH Hamiltonian with electron–phonon interactions has the following form [10]:

\[ H = H_\pi + H_{\pi \rightarrow \text{ph}}, \]  

where

\[ H_\pi = -t_0 \sum_{n,s} (c_{n+1,s}^\dagger c_{n,s} + c_{n,s}^\dagger c_{n+1,s}), \]  

(2.2)

describes the \( \pi \)-electron (e) hopping between sites \( n \) and \( n+1 \). \( t_0 \) is the hopping constant for an undimerized structure,

\[ H_{\pi \rightarrow \text{ph}} = \sum_{n} \left( \frac{p_{n}^2}{2M_{\text{CH}}} + \frac{K}{2} (u_{n+1} - u_{n})^2 \right) \]  

(2.3)

represents the lattice, i.e. the phonons (ph), \( M_{\text{CH}} \) is the mass of the CH group, \( K \) is the ‘spring’ constant, \( u_n \) is the deviation from the undimerized structure on site \( n \), and the interaction between these two is

\[ H_{\pi \rightarrow \text{ph}} = \alpha \sum_{n,s} (u_{n+1} - u_{n})(c_{n+1,s}^\dagger c_{n,s} + c_{n,s}^\dagger c_{n+1,s}), \]  

(2.4)

where \( \alpha \) is the e–ph interaction constant. Summing \( H_\pi \) and \( H_{\pi \rightarrow \text{ph}} \) one defines \( t_{n,n+1} = t_0 - \alpha (u_{n+1} - u_{n}) \).

2.1.2. Electron correlations. Electron correlations i.e., electron–electron interactions, are fundamental in the explanation of many physical phenomena displayed by conducting polymers, for example, the observed negative spin densities in trans-(CH)\(_x\), which demonstrates electronic correlations in these chains [21]. Since the SSH model (that is based only on electron–phonon interactions) gives zero spin density, other models that take into account electron correlations are naturally necessary. Besides, the inclusion of electron correlations is mandatory for the optical spectra of even polyenes [22].

The addition of a term describing electron interactions in the SSH Hamiltonian defines the Pariser–Parr–Pople (PPP) model [22,23], which provides an extension of the Hubbard model by properly accounting for the long-range character of the electron–electron (Coulomb) repulsion. Thus, we have

\[ H_{\text{PPP}} = H + H_{\pi \rightarrow \pi}, \]  

(2.5)

where \( H \) is the noninteracting Hamiltonian defined in equation (2.1) and \( H_{\pi \rightarrow \pi} \) is given by

\[ H_{\pi \rightarrow \pi} = \frac{1}{2}U \sum_{l} n_{l}n_{l} + \frac{1}{2} \sum_{l,l'} V_{l,l'}n_{l}n_{l'}, \]  

(2.6)

where \( U \) is an on-site Hubbard term, \( V_{l,l'} \) is an off-site interaction between electrons on sites \( l \) and \( l' \), and \( n_{l} = c_{l,\alpha}^\dagger c_{l,\alpha} + c_{l,\beta}^\dagger c_{l,\beta} - 1 \) is the net charge density on site \( l \) with spin \( \alpha \) (\( \beta \)). The prime in the last term implies \( l \neq l' \). The on-site correlations \( U \), and inter-site
Coulomb interactions $V_{l,l'}$ are, in principle, arbitrary, and generally Ohno’s formula [24] is employed [23, 25]:

$$V_{l,l'} = \frac{U}{\sqrt{1 + (r_{l,l'}/r_0)^2}}, \quad (2.7)$$

where $r_0 \approx 1.29 \text{ Å}, r_{l,l'}$ is the distance between sites $l$ and $l'$ in ångströms, and $U = 11.13–11.26$ eV. Thus, as pointed out in [23], the geometry and $U$ fix all inter-site interactions.

The influence of electronic correlations on structural and electronic properties of trans-(CH)$_x$, such as the ground-state energy, the amplitude of the bond alternation and the effective force constant for the bond-stretching mode, has been investigated using the Hamiltonian of equation (2.5) with $V_{l,l'} = 0$ but considering an effective $U$ [26]. The study of [26] finds a consistent modeling of trans-(CH)$_x$ if $U$ is chosen to be of the order of 7–9 eV.

Since the consideration of electron correlations is beyond the scope of the present work, in what follows we consider $U = V_{l,l'} = 0$.

### 2.1.3. The TLM continuum model Hamiltonian.

As pointed out in [11], in the weak coupling limit, only electrons of the Fermi surface with energy of order $\approx \Delta$ (the gap energy) are affected by the dimerization. Then it is reasonable to linearize the band structure in the vicinity of the points $\pm k_F$, where $k_F$ is the Fermi momentum. After the linearization, TLM obtained the continuum version of (2.1):

$$H = \frac{1}{2\pi \hbar v_F \lambda_{TLM}} \int dx \left[ \Delta^2(x) + \frac{\dot{\Delta}^2}{\Omega_0^2} \right] + \sum_s \int dx \psi_s^\dagger(x) [-i\hbar v_F \sigma_3 \partial_x + \Delta(x) \sigma_1] \psi^s(x), \quad (2.8)$$

where the constants above are related to those of the original SSH Hamiltonian as $\hbar v_F = 2t_0 \sigma, \lambda_{TLM} = (2\alpha)^2/2\pi K L_0, \Omega_0^2 = 4K/M_{CH}$ is a dimensionless coupling, $\sigma_x$ are the Pauli matrices, $\Delta(x)$ is a real gap related to lattice vibrations, and $\dot{\Delta}(x) \equiv d\Delta(x)/dt$. $\psi^s$ is a two-field component spinor $\psi^s = (\psi^s_L \psi^s_R)$, representing the ‘left moving’ and ‘right moving’ electrons close to their Fermi energy, respectively, where $s$ is an internal symmetry index (spin) that determines the effective degeneracy of the fermions, $s = 1 \equiv \uparrow$, and $s = 2 \equiv \downarrow$.

### 2.2. The model Lagrangian

The Lagrangian density of the TLM model in the adiabatic approximation ($\dot{\Delta}(x) = 0$) is given by

$$\mathcal{L}_{TLM} = \sum_s \psi_s^\dagger \left( i\hbar \partial_t - i\hbar v_F \gamma_5 \partial_x - \gamma_0 \Delta(x) \right) \psi^s - \frac{1}{2\pi \hbar v_F \lambda_{TLM}} \Delta^2(x), \quad (2.9)$$

where the gamma matrices are given in terms of the Pauli matrices, as $\gamma_0 = \sigma_1$, and $\gamma_5 = -\sigma_3$.

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The four-fermion Lagrangian density of the massless GN model \[12\] reads
\[
\mathcal{L}_{GN} = \sum_s \bar{\psi}^s (i\hbar \gamma_0 \partial_t - i\hbar v_F \gamma_1 \partial_x) \psi^s + \frac{\lambda_{GN} \hbar v_F}{2N} (\bar{\psi} \psi)^2, \tag{2.10}
\]
where \(\bar{\psi} = \psi^\dagger \gamma_0\) and \(\bar{\psi} \psi = \bar{\psi}^s \psi^s = \sum_{s=1}^N \bar{\psi}^s \psi^s\), and \(N\) is the number of flavors of Dirac fermions in the effective field theory. In the large \(N\) (mean-field) approximation, one obtains \[9,12\]
\[
\mathcal{L}_{GN} = \sum_s \bar{\psi}^s (i\hbar \partial_t - i\hbar v_F \gamma_0 \partial_x - \gamma_0 \Delta(x)) \psi^s - \frac{N}{2 \hbar v_F \lambda_{GN}} \Delta^2(x). \tag{2.11}
\]
Thus one sees that the equivalence between the TLM and the Gross–Neveu (GN) models is established by setting \(\lambda_{TLM} = (\lambda_{GN}/N\pi)\). Note that the fermion–lattice interaction in the equation above resembles the usual fermion–boson interaction in the quantum field theory context \[27\].

In order to consider the application of an external Zeeman magnetic field \(B_0\) parallel to the system and its effects, it is convenient to start by writing the grand canonical partition function associated with \(\mathcal{L}_{GN}\) in the imaginary time formalism \[28\]:
\[
Z = \int \mathcal{D} \bar{\psi} \mathcal{D} \psi \exp \left\{ \int_0^\beta d\tau \int dx \left[ \mathcal{L}_{GN} \right] \right\}, \tag{2.12}
\]
where \(\beta \equiv 1/k_BT\), \(k_B\) is the Boltzmann constant, and \(\mathcal{L}_{GN}\) is the Euclidean GN Lagrangian density:
\[
\mathcal{L}_{GN} = \sum_{s=1,2} \bar{\psi}^s \left[ -\gamma_0 \hbar \partial_t + i\hbar v_F \gamma_1 \partial_x - \Delta(x) + \gamma_0 \mu + \gamma_0 S_s \mu_B B_0 \right] \psi^s - \frac{1}{\hbar v_F \lambda_{GN}} \Delta^2(x), \tag{2.13}
\]
where \(\mu\) is the chemical potential, \(S_s = \pm 1/2\), \(g\) is the effective \(g\)-factor and \(\mu_B = e\hbar/2m \approx 5.788 \times 10^{-5} \text{ eV } \text{T}^{-1}\) is the Bohr magneton. The parallel magnetic field couples to the electrons’ spin and produces the Zeeman splitting energy term \(\Delta E = S_s g \mu_B B_0 \ [29,30]\) in equation (2.13). From the form of the Zeeman energy term in equation (2.13) we see that it can be added to the chemical potential, thus defining an effective chemical potential terms in the Lagrangian density of the form
\[
\sum_{s=1,2} \mu_s \bar{\psi}^s 0 \psi^s = \sum_{s=1,2} (\mu + S_s g \mu_B B_0) \bar{\psi}^s 0 \psi^s = \mu_1 \bar{\psi}^\dagger \psi_1 + \mu_1 \bar{\psi}^\dagger \psi_1, \tag{2.14}
\]
where \(\mu_1 = \mu + \delta \mu, \mu_1 = \mu - \delta \mu\), and \(\delta \mu \equiv (g/2) \mu_B B_0\). In \[27\] \(\mu = \mu_c\) has been chosen, such that when \(\delta \mu = B_0 = 0\) the system is in the symmetry restored phase. Thus we rewrite equation (2.13) as
\[
\mathcal{L}_{GN} = \sum_{s=1,2} \bar{\psi}^s \left[ -\gamma_0 \hbar \partial_t + i\hbar v_F \gamma_1 \partial_x - \Delta(x) + \gamma_0 \mu_s \right] \psi^s - \frac{1}{\hbar v_F \lambda_{GN}} \Delta^2(x), \tag{2.15}
\]
 Integrating over the fermion fields leads to
\[
Z = \exp \left\{ -\frac{\beta}{\hbar v_F \lambda_{GN}} \int dx \Delta^2(x) \right\} \Pi_{j=1}^2 \det D_j, \tag{2.16}
\]
where $D_j = -\gamma_0 \partial_x + i v_F \gamma_1 \partial_x + \gamma_0 \mu_j - \Delta(x)$ is the Dirac operator at finite temperature and density. Since $\Delta(x)$ is static, one can transform $D_j$ to the $\omega_n$ plane, where the $\omega_n = (2n + 1)\pi T$ are the Matsubara frequencies for fermions, yielding $D_j = (-i \omega_n + \mu_j)\gamma_0 + i v_F \gamma_1 \partial_x - \Delta(x)$. After using an elementary identity $\ln(\det(D_j)) = \text{Tr} \ln(D_j)$, one can define the bare effective action for the static $\Delta(x)$ condensate

$$S_{\text{eff}}[\Delta] = -\frac{\beta}{\hbar v_F \lambda_{\text{GN}}} \int dx \Delta^2(x) + 2 \sum_{j=1}^2 \text{Tr} \ln(D_j),$$

where the trace is to be taken over both Dirac and functional indices. The condition for finding the stationary points of $S_{\text{eff}}[\Delta]$ reads

$$\frac{\delta S_{\text{eff}}[\Delta]}{\delta \Delta(x)} = 0 = -\frac{2\beta}{\hbar v_F \lambda_{\text{GN}}} \Delta(x) + \frac{\delta}{\delta \Delta(x)} \left[ \sum_{j=1}^2 \text{Tr} \ln(D_j) \right].$$

The equation above is a complicated and generally unknown functional equation for $\Delta(x)$, whose solution has been investigated at various times in the literature [31]–[36]. Its solution is not only of academic interest, but has direct application in condensed matter physics, for example, in [7, 35], and in the present work.

3. Symmetry breaking and condensates at the mean-field level and beyond

The GN model in 1D has a discrete chiral symmetry which is dynamically broken by the non-perturbative vacuum [31]. As a result, there will be the generation of homogeneous and inhomogeneous $\Delta(x)$ condensates, as discussed below.

3.1. Homogeneous $\Delta(x)$ condensates

For a constant $\Delta$ field the Dirac operator reads $D_j = (-i \omega_n + \mu_j)\gamma_0 + i v_F \gamma_1 p - \Delta$, so the trace in equation (2.17) can be evaluated in a closed form for the asymmetrical ($\delta \mu \neq 0$) system [27]. From equation (2.16) one obtains the ‘effective’ potential $V_{\text{eff}} = -(k_B T/L) \ln Z$, where $L$ is the length of the system:

$$V_{\text{eff}}(\Delta, \mu_{\uparrow, \downarrow}, T) = \frac{1}{\hbar v_F \lambda_{\text{GN}}} \Delta^2 - k_B T \int_{-\infty}^{+\infty} \frac{dp}{2\pi \hbar} \left[ 2\beta E_p + \ln(1 + e^{-\beta E_p^+}) + \ln(1 + e^{-\beta E_p^-}) + \ln(1 + e^{-\beta E_{p+}^x}) + \ln(1 + e^{-\beta E_{p-}^x}) \right],$$

where $E_{p+}^\pm = E_p \pm \mu_{\uparrow, \downarrow}$, $E_p = \sqrt{v_F^2 p^2 + \Delta^2}$.

3.1.1. Zero temperature and zero chemical potentials. The first term in the integration in $p$ in equation (3.1), corresponding to the vacuum part ($\mu_{\uparrow, \downarrow} = T = 0$), is divergent. Introducing a momentum cutoff $\Lambda$ to regulate this part of $V_{\text{eff}}$, one obtains, after renormalization where the momentum cutoff is taken to infinity while maintaining finite and stable results, the following expression to the effective potential [12, 17]:

$$V_{\text{eff}}(\Delta) = \frac{\Delta^2}{\hbar v_F} \left( \frac{1}{\lambda_{\text{GN}}} - \frac{3}{2\pi} \right) + \frac{\Delta^2}{\pi \hbar v_F} \ln \left( \frac{\Delta}{m_F} \right),$$
where $m_F$ is an arbitrary renormalization scale, with the dimension of energy, introduced during the regularization process used to compute the appropriate momentum integrals. The minimization of $V_{\text{eff}}(\Delta)$ with respect to $\Delta$ gives $\Delta_0 = 0$ and the well-known result for the non-trivial gap [12]:

$$\Delta_0 = m_F e^{1 - \pi/\lambda_{\text{GN}}}.$$  (3.3)

This is the phenomenon of dynamical mass generation in the massless model. From this equation it is easy to see that with the experimentally measured $\Delta_0$ and $\alpha$, $t_0$ and $K$ which enter $\lambda_{\text{TLM}}$, one sets the value of $m_F$. Equation (3.2) can be expressed in a more convenient form in terms of $\Delta_0$ as

$$V_{\text{eff}}(\Delta) = \frac{\Delta^2}{2\pi\hbar v_F} \ln \left( \frac{\Delta^2}{\Delta_0^2} \right) - 1,$$  (3.4)

which is clearly symmetric under $\Delta \rightarrow -\Delta$, that generates the discrete chiral symmetry of the GN model. As we pointed out before, this discrete symmetry is dynamically broken and thus there is a kink solution interpolating between the two degenerate minima $\Delta = \pm \Delta_0$ of (3.4) at $x = \pm \infty$ [40]:

$$\Delta(x) = \Delta_0 \tanh(\Delta_0 x).$$  (3.5)

In section 3.2 we discuss the effects of space dependent $\Delta(x)$ condensates.

3.1.2. Zero temperature and finite chemical potentials. At finite chemical potential and in the zero-temperature limit, equation (3.1) reads

$$V_{\text{eff}}(\Delta, \mu_{\uparrow,\downarrow}) = \frac{1}{\hbar v_F \lambda_{\text{GN}}} \Delta^2 - 2 \int_0^\Lambda dp \frac{dE_p}{\pi\hbar} E_p + \int_0^{p_{\uparrow,F}} dp \frac{dE_p}{\pi\hbar} E_p^- + \int_0^{p_{\downarrow,F}} dp \frac{dE_p}{\pi\hbar} E_p^-, \quad (3.6)$$

where $p_{\uparrow,F} = (1/v_F)\sqrt{\mu_{\uparrow,F}^2 - \Delta^2}$ is the Fermi momentum of the spin-$\uparrow$ ($\downarrow$) moving electron. We integrate in $p$, observing that the renormalization is the same as before, to obtain [17]

$$V_{\text{eff}}(\Delta, \mu_{\uparrow,\downarrow}) = V_{\text{eff}}(\Delta) + \Theta_1 \mathcal{F}_1 + \Theta_2 \mathcal{F}_2,$$  (3.7)

where $V_{\text{eff}}(\Delta)$ is given by equation (3.4), $\Theta_{1,2} = \Theta(\mu_{\uparrow,\downarrow}^2 - \Delta^2)$ is the step function, defined as $\Theta(x) = 0$, for $x \leq 0$, and $\Theta(x) = 1$, for $x > 0$, and $\mathcal{F}_{1,2} \equiv (1/2\pi\hbar v_F) [\Delta^2 \ln((\mu_{\uparrow,\downarrow} + \sqrt{\mu_{\uparrow,\downarrow}^2 - \Delta^2})/\Delta) - \mu_{\uparrow,\downarrow} \sqrt{\mu_{\uparrow,\downarrow}^2 - \Delta^2}]$.

Although finite chemical potential is being considered now, the effective potential is unaffected if both $\mu_{\uparrow}$ and $\mu_{\downarrow}$ are smaller than $\Delta$, in which case it is reduced to that of equation (3.4). For $\mu_{\uparrow,\downarrow} > \Delta$ the ground state is determined by jointly finding $\Delta_0(\mu_{\uparrow,\downarrow})$, and the analyzing of the effective potential at the minimum, $V_{\text{eff}}(\Delta_0(\mu_{\uparrow,\downarrow}))$. Extremizing $V_{\text{eff}}(\Delta, \mu_{\uparrow,\downarrow})$ with respect to $\Delta$ yields the trivial solution $(\Delta = 0)$, and

$$\ln \left( \frac{\Delta}{\Delta_0} \right) + \Theta_1 \frac{G_1}{2} + \Theta_2 \frac{G_2}{2} = 0,$$  (3.8)

where $G_{1,2} \equiv \ln((\mu_{\uparrow,\downarrow} + \sqrt{\mu_{\uparrow,\downarrow}^2 - \Delta^2})/\Delta)$, and we have made use of equation (3.3) to eliminate $m_F$ in the gap equation above. Equation (3.8) cannot be solved in a closed form, for $\Delta > 0$. As before, we treat $\Delta > 0$ as a parameter, and make use of equation (3.8) to extremize $V_{\text{eff}}(\Delta, \mu_{\uparrow,\downarrow})$ with respect to $\Delta$.
form for \( \Delta \) as a function of \( \mu_{\uparrow,\downarrow} \). Nevertheless, for \( B_0 = 0 \) i.e., for \( \delta \mu = 0 \) which implies \( \mu_\uparrow = \mu_\downarrow = \mu \), it can be easily solved:

\[
\Delta_0(\mu) = \sqrt{\Delta_0(2\mu - \Delta_0)},
\]

where \( \Delta_0 \) is given by equation (3.3), and \((\Delta_0/2) \leq \mu \leq \Delta_0\). However, the analysis of \( V_{\text{eff}}(\Delta_0(\mu)) \) shows that \( \Delta_0(\mu) \) is a local maximum and the solution \( \Delta = \Delta_0 \) represents a global minimum of \( V_{\text{eff}}(\Delta, \mu) \) while \( \mu < \mu_c \) (where the critical chemical potential, \( \mu_c = (\Delta_0/\sqrt{2}) \), is obtained from \( V_{\text{eff}}(\Delta = 0, \mu_c) = V_{\text{eff}}(\Delta = \Delta_0, \mu_c) \)), with \( \Delta_0 = 0 \) representing a false minimum. When \( \mu \geq \mu_c \), \( \Delta(\mu \geq \mu_c) \) represents a local maximum and \( \Delta_0 = 0 \) is turned into a minimum through a first-order phase transition [15, 16], agreeing with experiment [8]. Thus, \( \Delta_0 \) as a function of the chemical potential in the absence of \( B_0 \) has the following expression:

\[
\Delta_0(\mu) = \Theta(\mu_c - \mu)\Delta_0.
\]

3.1.3. Magnetic properties at zero temperature. As mentioned before, the application of a static magnetic field to the system results in a Zeeman energy given by \( \Delta E = S_\epsilon g_B B_0 \), where \( S_\epsilon = \pm 1/2 \), \( g \approx 2 \) for trans-(CH)\(_x\) is the effective \( g \)-factor, \( \mu_B = e\hbar/2m \approx 5.788 \times 10^{-5} \text{ eV T}^{-1} \) is the Bohr magneton, \( m \) is the bare electron mass, and \( B_0 \) is the magnetic field strength. Then we have \( \delta \mu = |\Delta E| = (g/2)\mu_B B_0 \).

The number densities \( n_{\uparrow,\downarrow} = -(\partial/\partial \mu_{\uparrow,\downarrow})V_{\text{eff}}(\Delta, \mu_{\uparrow,\downarrow}) \) are obviously imbalanced due to the asymmetry between \( \mu_\uparrow \) and \( \mu_\downarrow \), and will depend on \( \delta \mu \). Before the critical asymmetry doping, \( \Delta_0(\delta \mu) = 0 \) and the densities read

\[
n_{\uparrow,\downarrow}(\delta \mu/\Delta_0 < 0.38) = \frac{1}{\pi \hbar v_F} \mu_{\uparrow,\downarrow}.
\]

For such a low imbalance, compared to the critical chemical potential asymmetry \( \delta \mu_c \), the total number density is the same as in the symmetric limit or, in other words, is independent of the applied magnetic field:

\[
n_T = n_\uparrow + n_\downarrow = 2n = \frac{2}{\pi \hbar v_F} \mu_c.
\]

In spite of that, there is a partial spin polarization

\[
\delta n = n_\uparrow - n_\downarrow = \frac{2}{\pi \hbar v_F} \delta \mu = \frac{2}{\pi \hbar v_F} \mu_B B_0.
\]

The zero-\( T \) Pauli magnetization of the polarized chain is defined as

\[
M = \mu_B \delta n = \frac{2\mu_B^2}{\pi \hbar v_F} B_0.
\]

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The magnetic susceptibility is given by

$$\chi = \frac{\partial M}{\partial B_0} = \frac{2\mu_B^2}{\pi \hbar v_F},$$

which is the well-known Pauli expression for the magnetic susceptibility for noninteracting electrons at zero temperature.

Increasing the asymmetry beyond the critical value $\delta\mu = (g/2)\mu_B B_{0,c}$, we find

$$n_\uparrow(\delta\mu/\Delta_0 > 0.38) = \frac{1}{\pi \hbar v_F} \sqrt{\mu_\uparrow^2 - \Delta^2},$$

where $\Delta$ in the equation above is the solution of equation (3.11) for a given $\delta\mu > \delta\mu_c$, and

$$n_\downarrow(\delta\mu/\Delta_0 > 0.38) = 0,$$

meaning that, effectively, there are only spin-$\uparrow$ electrons in the system i.e., the chain is fully polarized. The magnetization is now

$$M_{fp} = \mu_B n_\uparrow = \frac{\mu_B}{\pi \hbar v_F} \sqrt{\mu_\uparrow^2 - \Delta^2},$$

which also depends on the external magnetic field $B_0$ through $\Delta$. The results for the zero-temperature magnetization of a (CH)$_x$ wire under $B_0$ are displayed in figure 1.

### 3.1.4. Finite temperature and finite chemical potentials

The effects of finite temperature and density have been taken into account in the symmetric GN model ($\delta\mu = 0$) by several authors. See, for instance, [15, 41, 42] and references therein.

We can rewrite $V_{\text{eff}}(\Delta, \mu_{\uparrow,\downarrow}, T)$ as

$$V_{\text{eff}}(\Delta, \mu_{\uparrow,\downarrow}, T) = V_{\text{eff}}(\Delta) + V_{\text{eff}}(\mu_{\uparrow,\downarrow}, T),$$

where

$$V_{\text{eff}}(\mu_{\uparrow,\downarrow}, T) = -k_B T \int_0^{\infty} \frac{dp}{\pi \hbar} \left[ \ln(1 + e^{-\beta E_\uparrow}) + \ln(1 + e^{-\beta E_\downarrow}) \right]$$

$$+ \ln(1 + e^{-\beta E_\uparrow}) + \ln(1 + e^{-\beta E_\downarrow}).$$

Figure 1. Schematic representation of the spin orientations in the three possible situations with respect to the actuation of a Zeeman external constant magnetic field parallel to a (CH)$_x$ wire. In the first line, $B = 0$ and consequently $M = 0$. In the second line $B < B_{0,c} = 2\delta\mu_c/g\mu_B$ implying a net magnetization of the wire. Finally, when $B \geq B_{0,c}$ the wire is fully magnetized.
Since we cannot calculate expression (3.21) in a closed form, we shall use a high temperature expansion to evaluate it. Using the function
\[
I(a, b) = \int_0^\infty dx \left[ \ln(1 + e^{-\sqrt{a^2 + b^2} - b}) + \ln(1 + e^{-\sqrt{a^2 + a^2 + b}}) \right],
\] (3.22)
where \(a = \Delta/k_B T\), and \(b = \mu/k_B T\), which can be expanded in the high temperature limit, \(a \ll 1\) and \(b \ll 1\), yielding, up to order \(a^4\) and \(b^2\) [44],
\[
I(a \ll 1, b \ll 1) = \frac{\pi^2}{6} + \frac{b^2}{2} - \frac{a^2}{2} \ln \left( \frac{\pi}{a} \right) - \frac{a^2}{4}(1 - \gamma_E)
- \frac{7\xi(3)}{8\pi^2} a^2 \left( b^2 + \frac{a^2}{4} \right) + \frac{186\xi(5)}{128\pi^4} b^2 a^4 + O(a^2b^4),
\] (3.23)
where \(\gamma_E \approx 0.577 \ldots\) is the Euler constant and \(\xi(n)\) is the Riemann zeta function, having the values \(\xi(3) \approx 1.202\) and \(\xi(5) \approx 1.037\). With the equation above, together with equation (3.2), the high temperature asymmetrical effective potential is written as
\[
V_{\text{eff}}(\Delta, \mu_{\uparrow, \downarrow}, T) \equiv V_{\text{eff}} = \frac{\Delta^2}{\pi \hbar v_F} \left[ \ln \left( \frac{\pi k_B T}{\Delta_0} \right) - \gamma_E \right] - \frac{\pi}{3\hbar v_F}(k_B T)^2
- \frac{1}{2\pi \hbar v_F} \left[ \mu_\uparrow^2 + \mu_\downarrow^2 - \frac{7\xi(3)}{8\pi^2} \frac{\Delta^4}{(k_B T)^2} \right]
- \frac{7\xi(3)}{4\pi^2} \left( \mu_\uparrow^2 + \mu_\downarrow^2 \right) \frac{\Delta^2}{(k_B T)^2}
+ \frac{186\xi(5)}{64\pi^4} \left( \mu_\uparrow^2 + \mu_\downarrow^2 \right) \frac{\Delta^4}{(k_B T)^4}.\]
(3.24)
The equation above may be rearranged in the form of a Ginzburg–Landau (GL) expansion of the grand potential density, which is appropriate to the analysis of the phase diagram in the region near the tricritical point:
\[
V_{\text{eff}} = \alpha_0 + \alpha_2 \Delta^2 + \alpha_4 \Delta^4,
\] (3.25)
where
\[
\alpha_0(\mu_{\uparrow, \downarrow}, T) = -\frac{1}{2\pi \hbar v_F} \left[ \mu_\uparrow^2 + \mu_\downarrow^2 \right] - \frac{\pi}{3\hbar v_F}(k_B T)^2,\]
(3.26)
\[
\alpha_2(\mu_{\uparrow, \downarrow}, T) = \frac{1}{\pi \hbar v_F} \left[ \ln \left( \frac{\pi k_B T}{e^{\gamma_E} \Delta_0} \right) + \frac{7\xi(3)}{8\pi^2} \left( \mu_\uparrow^2 + \mu_\downarrow^2 \right) \right],\]
\[
\alpha_4(\mu_{\uparrow, \downarrow}, T) = -\frac{1}{32\pi^3 \hbar v_F(k_B T)^2} \left[ -14\xi(3) + \frac{186\xi(5)}{4\pi^2} \left( \mu_\uparrow^2 + \mu_\downarrow^2 \right) \right].\]
(3.27)
Extremizing \(V_{\text{eff}}\) we find the trivial solution \((\Delta = 0)\) and the chemical potential and temperature dependent gap equation
\[
\Delta_0(\mu_{\uparrow, \downarrow}, T)^2 = -\frac{\alpha_2}{2\alpha_4},\]
(3.28)
which has meaning only if the ratio \((\alpha_2/\alpha_4)\) is negative. Besides, a stable configuration (i.e., bounded from below) requires, up to this order, \(\alpha_4 > 0\). At the minimum, \(V_{\text{eff}}\) reads
\[
V_{\text{eff, min}} = \alpha_0 - \frac{\alpha_2^2}{4\alpha_4}.\]
(3.29)
The critical temperature $T_c$ is the temperature at which the coefficient of $\Delta^2$ vanishes i.e. $\alpha_2 = 0$, or

$$
\ln \left( \frac{\pi k_B T_c}{e^{\gamma} \Delta_0} \right) + \frac{7\xi(3)}{8\pi^2} \frac{(\mu_1^2 + \mu_1^2)}{(k_B T_c)^2} = 0,
$$

(3.30)

where $T_c = T_c(\mu_1, \mu_1)$. As will become clear below, the equation above defines a second-order transition line separating the non-metallic ($\Delta \neq 0$) and metallic phases ($\Delta = 0$). At $\mu_1 = \mu_1 = 0$, we recover the well-known result for the temperature at which the discrete chiral symmetry is restored [46]:

$$
T_c(\mu_1 = \mu_1 = 0) \equiv T_c(0) = \frac{e^{\gamma} \Delta_0}{\pi k_B},
$$

(3.31)

In order to find $T_c(\mu_1, \mu_1)$ we define dimensionless variables $\nu = (7\xi(3)/8\pi^2)((\mu_1^2 + \mu_1^2)/(k_B T_c(0))^2)$ and $t = (T/T_c(0))$, and with the help of equation (3.31) we rewrite the LHS of equation (3.30) as

$$
y(t) = \ln(t) + \frac{\nu}{t^2}.
$$

(3.32)

The zeros of $y(t)$ for a given $\nu$, i.e., for a given $\mu_1^2 + \mu_1^2$, are the respective $T_c$. This defines the (second-order) $T_c$ versus $\mu_1^2 + \mu_1^2$ phase diagram. A graphical inspection of $y(t)$ [47] shows that there is no solution for this function for $\nu$ above a certain value, that we define as $\nu_c$. Besides, at $\nu_c$ we have $y = y' = 0$. These two equations give $t_{c}$ and $\nu_c$ for the tricritical point $P_{c} = (\nu_c, t_c)$. Strictly speaking, $y$ and $y'$ are associated with the coefficients of the second-order and fourth-order terms of the effective potential expanded in powers of $\Delta$ [48]. Solving the equations $y = 0$ and $y' = 0$ self-consistently (which is equivalent to solving $\alpha_2 = \alpha_4 = 0$), we obtain the tricritical point analytically:

$$
\nu_c = \frac{7\xi(3) (\mu_1^2 + \mu_1^2)}{8\pi^2} = \frac{1}{2 \nu}, \quad t_c = \frac{T_c}{T_c(0)} = \sqrt{\frac{2\nu_c}{\nu(c)}} = \sqrt{\frac{1}{\nu}}.
$$

(3.33)

For $\nu$ above a certain value and less than $\nu_c$, the function $y$ presents two solutions for $T_c$. However, the lower of these always corresponds to unstable solutions. The second-order transition curve, defined as the line starting at the point $(0, T_c(0))$ and ending at the point $((\mu_1^2 + \mu_1^2), T_c)$, comes simply from the solution of the gap equation. This curve, shown in figure 2, represents a system at finite temperature where the chemical potentials $\mu_1^2 + \mu_1^2 = 2(\bar{\mu}^2 + \delta \mu^2)$ start from zero and increases until $((\mu_1^2 + \mu_1^2), T_c)$. Note that $\bar{\mu}^2 + \delta \mu^2$ is zero if and only if $\bar{\mu}^2$ and $\delta \mu^2$ are both zero. It is well known that below the tricritical point one has to properly minimize the effective potential rather than using the gap equation as the transition becomes first order. Thus equation (3.30) cannot be used for finding $T_c$ below $P_{c}$ since this equation is valid only for the second-order transition. In this case $T_c$ has to be found numerically, through the equality $V_{eff}(T_c, \mu_1, \mu_1, \Delta = \Delta_{min}) = V_{eff}(T_c, \mu_1, \mu_1, \Delta = 0)$, where $\Delta_{min}$ is the non-trivial minimum of $V_{eff}$.

The number densities $n_{1,1} = -\langle \partial / \partial \mu_{1,1} \rangle V_{eff}(T, \mu_{1,1}, \Delta)$ read

$$
n_{1,1}(T, \mu_{1,1}, \Delta) = \int_0^\infty \frac{dp}{\pi \hbar} \left[ n_k(E_{1,1}^+) - n_k(E_{1,1}^-) \right],
$$

(3.34)

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Figure 2. The phase diagram $t = (T/T_c(0))$ as a function of $\nu = (7\xi(3)/8\pi^2)((\mu_1^2 + \mu_2^2)/(k_B T_c(0))^2)$, from equation (3.30). The second-order transition line ends at the tricritical point $P_{tc} = ((1/2e), (1/\sqrt{e}))$. Below this point the transition is of first order.

where $n_k(E_{\uparrow,\downarrow}^\pm) = 1/(e^{\beta E_{\uparrow,\downarrow}^\pm} + 1)$ is the Fermi distribution function. The density difference

$$\delta n = n_\uparrow - n_\downarrow \quad (3.35)$$

is zero if $\delta \mu = (g/2)\mu_B B_0 = 0$, at any temperature, since in this case we have the equalities $n_k(E_{\uparrow}^+) = n_k(E_{\downarrow}^+)$, and $n_k(E_{\uparrow}^-) = n_k(E_{\downarrow}^-)$. The physical meaning of these results is that at zero external Zeeman magnetic field, the $\uparrow$ (up) and $\downarrow$ (down) electrons of the conduction $(\uparrow)$ band have the same density, and the same is so for the electrons of the valence $(\downarrow)$ band.

In the high temperature regime, the number densities are given by

$$n_{\uparrow,\downarrow}(T) = \frac{1}{\pi\hbar v_F} \left[ 1 - \frac{7\xi(3)}{4\pi^2} \frac{\Delta^2}{(k_B T)^2} \right] \mu_{\uparrow,\downarrow}. \quad (3.36)$$

In the high temperature limit the total number density, $n_T(T) = n_\uparrow(T) + n_\downarrow(T)$, is independent of the applied field, as happens at zero $T$:

$$n_T(T) = \frac{2}{\pi\hbar v_F} \left[ 1 - \frac{7\xi(3)}{4\pi^2} \frac{\Delta^2}{(k_B T)^2} \right] \bar{\mu}, \quad (3.37)$$

and for the density difference we obtain

$$\delta n_{\text{high}}(T, \delta \mu) = \frac{2}{\pi\hbar v_F} \left[ 1 - \frac{7\xi(3)}{4\pi^2} \frac{\Delta^2}{(k_B T)^2} \right] \delta \mu, \quad (3.38)$$

which, as we have observed before, is clearly zero if $B_0 = \delta \mu = 0$. Since the densities have to be evaluated at the minimum of the effective potential\(^1\), we use equation (3.28) in the

---

\(^1\) Remembering that the thermodynamical potential per volume is defined as the free energy density (or effective potential in the field theory language that we are using here) at its minimum, $\Omega(T, \mu_{\uparrow,\downarrow}) = V_{\text{eff}}(T, \mu_{\uparrow,\downarrow}, \Delta_{\text{min}})$.
equation above and find the temperatures at which the densities and, consequently, the density difference vanish. These temperatures are the solutions of
\[
\gamma_E - \frac{1}{2} + \ln \left( \frac{\Delta_0}{\pi k_B T_c^*} \right) - \frac{7\xi(3) (\mu_1^2 + \mu_2^2)}{8\pi^2 (k_B T_c^*)^2} = 0,
\]
(3.39)
where \( T_c^* = T_c^*(\mu_1, \mu_1) \). As for the gap parameter, the equation above defines the second-order line for the densities and the density imbalance. At \( \mu_1 = \mu_\uparrow = 0 \), we get
\[
T_c^*(\mu_\uparrow = \mu_\downarrow = 0) \equiv T_c^*(0) = \frac{e^{\gamma_E} - 1}{\pi} \Delta_0 k_B.
\]
(3.40)
It is very easy to see that \( T_c^*(0) = (T_c(0)/\sqrt{c}) \), which coincides with \( T_{ic} \), where \( T_{ic} \) is given by equation (3.33). Proceeding as before we find
\[
\nu_{tc}^* = \frac{7\xi(3) (\mu_1^2 + \mu_2^2)}{8\pi^2 (k_B T_c(0))^2} = \frac{1}{2e^2}, \quad t'_{tc} = \frac{T_{tc}^*}{T_c^*(0)} = \sqrt{2\nu_{tc}^*} = \frac{1}{e},
\]
(3.41)
defining the tricritical point for the densities, total density and density imbalance second-order curves.

Let us now verify the possibility of a fully polarized state at finite temperature. It would be possible with a magnetic field with an intensity such that \( n_1 \) in equation (3.36) vanishes. In this case \( \mu_1 = \bar{\mu} - \delta \mu_\uparrow = \mu_\uparrow - (g/2) \mu_B B_{0,e} = 0 \), or
\[
B_{0,e} = \frac{2\mu_c}{g\mu_B}.
\]
(3.42)

3.1.5. Magnetic properties at high temperature. The Pauli magnetization of the chain in the high temperature limit has the following expression:
\[
M_{high}^\uparrow(T) = \mu_B \delta n_{high}^\uparrow T(T) = \frac{2\mu_B}{\pi \hbar v_F} \left[ 1 - \frac{7\xi(3)}{4\pi^2} \frac{\Delta_0^2}{(k_B T)^2} \right] \delta \mu
\]
\[
= \frac{g\mu_B^2}{\pi \hbar v_F} \left\{ 1 - 2 \left[ \ln \left( \frac{T}{T_c(0)} \right) + \frac{7\xi(3)}{8\pi^2} \frac{\Delta_0^2 (k_B T)^2}{(k_B T)^2} \right] \right\} B_0,
\]
(3.43)
where \( T_c(0) \) is given by equation (3.31) and we have made use of equation (3.28) to leading order in \( \mu_1^2 + \mu_2^2)/(k_B T)^2 \). The second-order line where the magnetization vanishes is the same as the one given by equation (3.39). With \( M_{high}^\uparrow(T) \) we are in a position to obtain the magnetic susceptibility in this regime:
\[
\chi_{high}^\uparrow(T) = \frac{\partial M_{high}^\uparrow(T)}{\partial B_0} = \chi(0) - \chi(T),
\]
(3.44)
where
\[
\chi(0) = \frac{g\mu_B^2}{\pi \hbar v_F},
\]
(3.45)
is the zero-temperature Pauli magnetic susceptibility for noninteracting electrons given by equation (3.16), and
\[
\chi(T) = \frac{2g\mu_B^2}{\pi \hbar v_F} \left[ \ln \left( \frac{T}{T_c(0)} \right) + \frac{7\xi(3)}{4\pi^2 (k_B T)^2} \left( \mu_1^2 + \frac{3}{4} g^2 \mu_B^2 B_0^2 \right) \right].
\]
(3.46)
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The function $\chi_{\text{high}}(T)$ also behaves at finite temperature like the densities and the magnetization, with a second-order transition up to a tricritical point given by equation (3.41). Below this point the transition is again of first order.

Note that despite the full polarization, at $B_{0,c}$ the magnetization is given by exactly the same expression as was shown in equation (3.43). With the help of equation (3.36) we find

$$M_{\text{high}}(T,c) = \mu_B n_\uparrow(T) = \mu_B \left[ 1 - \frac{7 \xi(3) \Delta^2}{4 \pi^2 (k_B T)^2} \right] (\mu_c + \delta \mu_c)$$

$$= \frac{g \mu_B^2}{\pi \hbar v_F} \left\{ \ln \left( \frac{T}{T_c(0)} \right) + \frac{7 \xi(3) (\mu_\uparrow^2 + \mu_\downarrow^2)}{8 \pi^2 (k_B T)^2} \right\} B_{0,c}.$$  (3.47)

This shows that this function is indeed continuous for $0 \leq B_0 \leq B_{0,c}$.

3.2. Inhomogeneous $\Delta(x)$ condensates.

Since we consider the addition of a chemical potential (i.e., doping) in the theory representing a Peierls distorted material like TPA, and the effects of a Zeeman magnetic field on these materials, some important remarks are in order. It is well known that doping in conducting polymers with degenerate ground states results in lattice deformation, or nonlinear excitations, such as kink solitons and polarons, meaning that $\Delta(x)$ can vary in space [7,52,53]. Therefore, one may expect not only homogeneous-like configurations (as considered in section 3.1), but also that the inclusion of these excitations in any theoretical calculation in this model should be considered. In this context, within the GN field theory model that we are considering, by taking into account kink-like configurations in the large $N$ approximation, the authors of [33]–[36] found evidence for a crystalline phase that shows up in the extreme $T \sim 0$ and large $\mu$ part of the phase diagram, while the other extreme of the phase diagram, for large $T$ and small $\mu$, seemed to remain identical to the usual large $N$ results for the critical temperature and tricritical points, which are well-known results [15] for the GN model. The restoration of the broken discrete chiral symmetry of the massless GN model, which is signaled when the kink–antikink crystalline condensate [34,37,38] transforms into the kink crystal, is explained when an exotic supersymmetric structure is properly considered [39].

To take into account the effects of inhomogeneous configurations in the GL expansion of the grand potential density, let us write equation (3.25) in terms of $\Delta(x)$ and its derivatives up to $\alpha_4$ [33]–[36]:

$$V_{\text{eff}}(x) = \alpha_0 + \alpha_2 \Delta(x)^2 + \alpha_4 [\Delta(x)^4 + \Delta(x)^2],$$  (3.48)

where $\Delta(x)' \equiv d\Delta(x)/dx$. A straightforward variational calculation gives the following condition for the minimization of the free energy $E = \int V_{\text{eff}}(x) \, dx$:

$$\Delta(x)'' - 2\Delta(x)^3 - \frac{\alpha_2}{\alpha_4} \Delta(x) = 0.$$  (3.49)

The general solution of an equation of the form

$$\Delta(x)'' - 2\Delta(x)^3 + (1 + \varsigma) \Delta_0^2 \Delta(x) = 0,$$  (3.50)

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can be written as [36]

\[ \Delta(x, \varsigma) \equiv \Delta(x) = \Delta_0 \sqrt{\varsigma \text{ sn}(\Delta_0 x; \varsigma)}, \tag{3.51} \]

where \( \text{sn} \) is the Jacobi elliptic function with the real elliptic parameter \( 0 \leq \varsigma \leq 1 \). The \( \text{sn} \) function has period \( 2K(\varsigma) \), where \( K(\varsigma) \equiv \int_0^{\pi/2} [1 - \varsigma \sin^2(z)]^{-1/2} \, dz \) is the complete elliptic integral of first kind. At \( T = 0 \) and finite density (or \( \mu \)), the \( \varsigma \) parameter can be determined by a variational procedure yielding an average fermion density dependent transcendental equation for \( \varsigma \), which can be solved in the low and high density limits [35]. At finite \( T \) and \( \mu \), the \( \varsigma \) parameter can be determined within the Schnetz, Thies and Urlichs ansatz to solve the inhomogeneous gap parameter problem, together with the scale factor \( A \), by a numerical minimization of the renormalized grand canonical potential [33].

\( \Delta(x) \) in (3.51) represents an array of real kinks. When \( \varsigma = 1 \) equation (3.51) is reduced to the single-kink condensate given in equation (3.5). By a direct comparison between equations (3.49) and (3.50) one can easily identify the scale parameter \( \Delta_0 \) at high \( T \) (i.e. \( T \) near \( T_c \)) as

\[ \Delta_0 = \sqrt{\left( \frac{\alpha_2}{\alpha_4} \right) \frac{1}{1 + \varsigma}} \equiv \Delta_0(\varsigma). \tag{3.52} \]

Since \( (1 + 1 + \varsigma) > 0 \), the solution for inhomogeneous condensates has physical meaning only if the ratio \( (\alpha_2/\alpha_4) \) is negative, as in the case of homogeneous condensates.

In order to see the effects of equation (3.51) in the grand potential density, we add the term \(-\alpha_4 \frac{1}{3} (\Delta(x)^2)^{\prime\prime}\) to \( V_{eff}(x) \) in equation (3.48). It is easy to see that this term does not alter the solution for the minimum of the free energy, equation (3.49), but allows the use of the following important identities supported by the solution in (3.50):

\[
\begin{align*}
(\Delta(x)^{\prime})^2 &= \Delta^4(x) - (1 + \varsigma)\Delta_0^2 \Delta(x)^2 + \varsigma \Delta_0^4, \\
(\Delta(x)^{\prime\prime})^2 &= 6\Delta^4(x) - 4(1 + \varsigma)\Delta_0^2 \Delta(x)^2 + 2\varsigma \Delta_0^4. \tag{3.53}
\end{align*}
\]

With the equations above, we can write the \( x \) dependent grand potential density as

\[ V_{eff}(x) = \alpha_0 + \alpha_2 \Delta(x)^2 + \alpha_4 \frac{1}{3} \left[ (1 + \varsigma)\Delta_0^2 \Delta(x)^2 + \varsigma \Delta_0^4 \right]. \tag{3.54} \]

Averaging over one period, it is found [36] that \( \langle \Delta(x)^2 \rangle = (1 - E(\varsigma)/K(\varsigma))\Delta_0^2 \), where \( E(\varsigma) \) is the complete elliptic integral of second kind. The ratio \( E(\varsigma)/K(\varsigma) \) is a smooth function of \( \varsigma \) interpolating monotonically between 0 and 1. Thus we can write

\[ \langle V_{eff}(x) \rangle = \alpha_0 + A_2 \Delta_0^2 + A_4 \Delta_0^4, \tag{3.55} \]

where

\[ A_2 = \alpha_2 \left( 1 - \frac{E(\varsigma)}{K(\varsigma)} \right), \quad A_4 = \alpha_4 \frac{1}{3} \left[ \varsigma + (1 + \varsigma) \left( 1 - \frac{E(\varsigma)}{K(\varsigma)} \right) \right]. \tag{3.56} \]

As we will see next, with the consideration of inhomogeneous \( \Delta(x) \) condensates we obtain very interesting results. This generalizes the analysis of the grand potential density, such that the results obtained in subsection \( A \) for homogeneous condensates are particular cases which are obtained when specific values of the elliptic parameter \( \varsigma \) are taken:

(1) For \( \varsigma = 0 \), \( E(\varsigma = 0)/K(\varsigma = 0) = 1 \), which implies \( A_2 = A_4 = 0 \), and the grand potential density is that of the metallic phase, for which \( \Delta = 0 \) and \( V_{eff} = \alpha_0 \).

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(II) For $\varsigma = 1$, $E(\varsigma = 1)/K(\varsigma = 1) = 0$, so the grand potential density is that of the homogeneous case, equation (3.25), at the non-trivial minimum $\Delta_0$: $V_{\text{eff}} = \alpha_0 + \alpha_2\Delta_0^2 + \alpha_4\Delta_0^4$.

Besides, we find that:

(III) For $0 < \varsigma < 1$, the grand potential density is that of equation (3.55) which, as expected, is the interpolation of the two previous ones.

And finally, we find that the tricritical point is ‘stationary’ under the application of an external Zeeman magnetic field on CH chains:

(IV) For any $0 < \varsigma \leq 1$ it is easy to see from equation (3.55) that the tricritical point is still found for $\alpha_2 = \alpha_4 = 0$. These coefficients are $\mu, \tau$ dependent and were not affected by the space dependence of the condensate $\Delta(x)$, as seen in the symmetric case ($\delta\mu = B_0 = 0$) [33]–[36]. The novelty is that the location of the tricritical point of the TPA phase diagram under the influence of an external Zeeman magnetic field is also unaltered even considering an $x$ dependent grand potential density. This happens because in the high temperature limit the influence of the Zeeman field is not sufficient to change the position of the tricritical point.

3.3. The Gross–Neveu model beyond the mean-field approximation

We now investigate the GN model beyond the mean-field or large $N$ approximation employing the optimized perturbation theory (OPT). The OPT is a method for taking into account non-perturbative contributions to the mean-field results, which are of crucial importance for recovering the reliability of perturbation theory at finite temperature, mainly in theories displaying thermodynamical phase transitions [43]. For a better description of the implementation of the OPT procedure, please see [44,49]. The OPT is closely related to the optimized expansion (OE) method. Like the OPT, the OE is an alternative non-perturbative technique which also allows one to go beyond the framework of the standard perturbative expansion [45].

Applying the usual OPT interpolation prescription to the original Lagrangian density given by equation (2.10), we define the interpolated theory:

$$L_{\text{GN}}^\delta(\psi, \bar{\psi}) = \sum_s \bar{\psi}^s (i\hbar\gamma_0 \partial_t - i\hbar v_F \gamma_1 \partial_x) \psi^s - \eta(1 - \delta)\bar{\psi}\psi + \delta \lambda_{\text{GN}}^{\delta} \frac{N}{2}\hbar v_F (\bar{\psi}\psi)^2. \quad (3.57)$$

It is easy to verify that at $\delta = 0$ we have a theory of free fermions, and the original theory is recovered for $\delta = 1$. $\eta$ is an arbitrary mass parameter. Now, by re-introducing the scalar field $\Delta$, which can be achieved by adding the quadratic term corresponding to a Hubbard–Stratonovich trick:

$$-\frac{\delta N}{2\hbar v_F \lambda_{\text{GN}}} \left( \Delta + \lambda_{\text{GN}}^{\delta} \frac{N}{2}\hbar v_F \bar{\psi}\psi \right)^2, \quad (3.58)$$

to $L_{\text{GN}}^\delta(\psi, \bar{\psi})$, one obtains the interpolated model corresponding to the original TLM model given by equation (2.9),

$$L_{\text{GN}}^\delta = \sum_{s=1,2} \bar{\psi}^s (i\hbar\gamma_0 \partial_t - i\hbar v_F \gamma_1 \partial_x) \psi^s - \delta \Delta \bar{\psi}\psi - \eta(1 - \delta)\bar{\psi}\psi - \frac{\delta N}{2\hbar v_F \lambda_{\text{GN}}} \Delta^2. \quad (3.59)$$

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Introducing the chemical potentials as before and considering the actuation of the Zeeman field, as explained below equation (2.12), we write

\[ L^δ GN = \sum_{s=1,2} \bar{\psi}^s \left[ -\gamma_0 \hbar \partial_x + i \hbar v_F \gamma_1 \partial_x + \gamma_0 \mu_s \right] \psi^s - \delta \Delta \bar{\psi}\psi - \eta (1 - \delta) \bar{\psi}\psi - \frac{\delta N}{2 \hbar v_F \lambda_{GN}} \Delta^2. \]

(3.60)

Since equation (3.60) in the limit \( \delta \mu \to 0 \) is the same model as was already studied in [44], we do not repeat all of the details related to the free energy density derivation here, where only the main steps and results relevant for our application to the CH chains will be presented.

Generally, the OPT method can be implemented as follows. Any physical quantity, \( F^{(k)} \), is perturbatively computed from the interpolated model, up to some finite order \( k \) in \( \delta \), which is formally used only as a bookkeeping parameter which is set to the unity, at the end of the calculation. But in this process any (perturbative) result at order \( k \) in the OPT remains \( \eta \) dependent. This arbitrary \( (a \ priori) \) parameter is then fixed by a variational method that then generates non-perturbative results, in the sense that it resums to all orders a certain class of perturbative contributions through self-consistent equations. Such an optimization method is known as the principle of minimal sensitivity (PMS) and amounts to requiring that \( F^{(k)} \) be evaluated at the point where it is less sensitive to this parameter. This criterion translates into the variational relation [50]

\[ \frac{dF^{(k)}}{d\eta} \bigg|_{\delta=1, \eta=\bar{\eta}} = 0. \]

(3.61)

The optimum value \( \bar{\eta} \) that satisfies equation (3.61) must be a function of the original parameters, including the couplings, thus generating ‘non-perturbative’ results. In our case, we are interested in evaluating the optimized free energy at finite temperature and density for the scalar field, \( \Delta \), once the fermions have been integrated out.

3.3.1. The optimized free energy density. We generalize to the asymmetrical case Landau’s free energy density (or effective potential, in the language of quantum field theories) to order \( \delta \), that has been evaluated in [44] using usual functional and diagrammatic techniques. The result is

\[
\mathcal{F}(\Delta, \eta, T, \mu_{\uparrow, \downarrow}) = \delta \frac{N \Delta^2}{2 \lambda_{GN} v_F \hbar} - \frac{N}{2 \pi v_F \hbar} \times \left\{ \eta^2 \left[ \frac{1}{2} + \ln \left( \frac{m_F}{\eta} \right) \right] + (kT)^2 \left[ I_1(\eta, \mu_{\uparrow}, T) + I_1(\eta, \mu_{\downarrow}, T) \right] \right\}
+ \delta \frac{N \eta(\eta - \Delta)}{\pi v_F \hbar} \left[ \ln \left( \frac{m_F}{\eta} \right) - \frac{1}{2} (I_2(\eta, \mu_{\uparrow}, T) + I_2(\eta, \mu_{\downarrow}, T)) \right]
+ \delta \frac{\lambda_{GN}}{4 \pi^2 v_F \hbar} \eta^2 \left[ \ln \left( \frac{m_F}{\eta} \right) - \frac{1}{2} (I_2(\eta, \mu_{\uparrow}, T) + I_2(\eta, \mu_{\downarrow}, T)) \right]^2
+ \delta \frac{\lambda_{GN}}{4 \pi^2 v_F \hbar} \frac{1}{2} (kT)^2 \left[ I_3^2(\eta, \mu_{\uparrow}, T) + I_3^2(\eta, \mu_{\downarrow}, T) \right].
\]

(3.62)
where the functions $I_1$, $I_2$ and $I_3$ are given respectively by

$$I_1(\eta, \mu, T) = \int_0^\infty dx \left\{ \ln \left[ 1 + e^{-(x^2 + \eta^2/2kT)^2} \right] + \ln \left[ 1 + e^{-(x^2 + \eta^2/2kT)^2 + \mu/kT} \right] \right\}, \quad (3.63)$$

$$I_2(\eta, \mu, T) = \int_0^\infty \frac{dx}{\sqrt{x^2 + \eta^2/2kT}} \left[ \frac{1}{e^{(x^2 + \eta^2/2kT)^2 + \mu/kT} + 1} \right] \left. + \frac{1}{e^{(x^2 + \eta^2/2kT)^2 - \mu/kT} + 1} \right], \quad (3.64)$$

and

$$I_3(\eta, \mu, T) = \sinh \left( \frac{\mu}{kT} \right) \int_0^\infty \frac{dx}{\cosh \left( \sqrt{x^2 + \eta^2/2kT} \right)} + \cosh \left( \frac{\mu}{kT} \right). \quad (3.65)$$

In equation (3.62), $\Delta$ is the homogeneous (constant field) configuration for the scalar field discussed already in the section 3.1. In the computation performed in [44], the free energy density has been renormalized using the \textit{MS} scheme for dimensional regularization. For a direct comparison between our results and that of [44], we have adopted dimensional regularization in this section instead of the cutoff regularization that we employed in section 3.3. As will be clear soon, equation (3.62), evaluated at first order in the OPT, already takes into account corrections beyond the large $N$ (or mean-field) leading order result.

By optimizing equation (3.62) through the PMS condition, equation (3.61), we obtain the optimum value for the parameter $\eta = \bar{\eta}$, which is then re-inserted in equation (3.62), allowing us to compute the order parameter $\bar{\Delta}$ that minimizes the free energy. Using the PMS procedure we then obtain, from equation (3.62) at $\eta = \bar{\eta}$ and $\delta = 1$, the general result which factors into

$$\left[ y(\eta, \mu, T) + \eta \frac{d}{d\eta} y(\eta, \mu, T) \right] \left[ \eta - \Delta + \eta \frac{\lambda_{GN}}{2\pi N} \left[ y(\eta, \mu, T) \right] \right]_{\eta = \bar{\eta}} + \frac{(kT)^2 \lambda_{GN}}{4\pi N}$$

$$\times \left[ I_3(\eta, \mu, T) \frac{d}{d\eta} I_3(\eta, \mu, T) + I_3(\eta, \mu, T) \frac{d}{d\eta} I_3(\eta, \mu, T) \right]_{\eta = \bar{\eta}} = 0, \quad (3.66)$$

where we have defined the function

$$y(\eta, \mu, T) \equiv \ln \left( \frac{m_F}{\eta} \right) - \frac{1}{2} \left( I_2(\eta, \mu, T) + I_2(\eta, \mu, T) \right). \quad (3.67)$$

Note that when $N \rightarrow \infty$ in equation (3.66), one obtains the solution $\bar{\eta} = \Delta$ and the mean-field standard result is exactly reproduced, as it should be [44,51].

### 3.3.2. The gap energy at zero temperature and chemical potential beyond the mean-field level.

In order to perform a numerical analysis we must fix all parameters. This can be done by considering the gap energy. In the GN language the order parameter $\Delta$ is just the TLM gap parameter which, at $T = 0$ and $\mu = 0$, has been denoted as $\Delta_0$ in equation (3.3). At
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\( T = \mu = 0 \) we have that \( I_1 = I_2 = I_3 = 0 \), so equation (3.66) and \( d\mathcal{F}/d\Delta = 0 \) give, at order \( \delta \), respectively,

\[
\Delta = \bar{\eta} \left[ 1 + \frac{\lambda_{GN}}{2\pi N} \ln \left( \frac{m_F}{\bar{\eta}} \right) \right],
\]

and

\[
\Delta = \frac{\lambda_{GN}}{\pi} \bar{\eta} \ln \left( \frac{m_F}{\bar{\eta}} \right),
\]

Plugging \( \bar{\eta} \ln(m_F/\bar{\eta}) = \pi \Delta/\lambda_{GN} \) from equation (3.69) in (3.68) we find

\[
\Delta = \left( 1 - \frac{1}{2N} \right)^{-1} \bar{\eta}.
\]

Solving these equations self-consistently yields

\[
\bar{\eta}_{\delta}^1(T = \mu_{\uparrow,\downarrow} = 0) \equiv \bar{\eta}_{\delta}^1(0) = m_F e^{-\pi/\lambda_{GN}(1-1/2N)},
\]

and

\[
\Delta_{\delta}^1(T = \mu_{\uparrow,\downarrow} = 0) \equiv \Delta_{\delta}^1(0) = F(N)^{-1} m_F e^{-\pi/\lambda_{GN}F(N)},
\]

where \( F(N) = 1 - 1/2N \). As pointed out in [44], equation (3.72) explicitly includes corrections beyond large \( N \), as obtained from the OPT approach, in the mean-field result. More precisely, taking the mean-field approximation, \( N \to \infty \), in equation (3.72) and using the relation \( \lambda_{GN} = N \pi \lambda_{TLM} \), the OPT result exactly recovers the mean-field result for \( N = 2 \) [7], as expected [44,51]. Besides, we have that \( \Delta_{\delta}^1(0) \) in the limit \( N \to \infty \) reproduces equation (3.72) with an appropriate redefinition of the (arbitrary) renormalization scale \( m_F \).

It is worth mentioning that, usually, in a renormalizable quantum field theory, one can choose an arbitrary value for \( m_F \) and \( \lambda_{GN} \) will run with the scale appropriately, at a given perturbative order, so \( \Delta_0 \) remains scale invariant as dictated by the renormalization group [9].

3.3.3. The gap energy at zero temperature and finite chemical potential beyond the mean-field level. We start by taking the \( T \to 0 \) limit of the functions defined by equations (3.63)–(3.65) which appear in the free energy density, equation (3.62). In this limit, these equations read [44]

\[
\lim_{T \to 0} T^2 I_1(\eta, \mu, T) = -\frac{1}{2} \theta(\mu - \eta) \left[ \eta^2 \ln \left( \frac{\mu + \sqrt{\mu^2 - \eta^2}}{\eta} \right) - \mu \sqrt{\mu^2 - \eta^2} \right],
\]

\[
\lim_{T \to 0} I_2(\eta, \mu, T) = \theta(\mu - \eta) \ln \left( \frac{\mu + \sqrt{\mu^2 - \eta^2}}{\eta} \right),
\]

\[
\lim_{T \to 0} T^2 I_3(\eta, \mu, T) = \text{sgn}(\mu) \theta(\mu - \eta) \sqrt{\mu^2 - \eta^2}.
\]
Using equations (3.73)–(3.75) in the PMS equation, equation (3.66), we notice that it can be divided into two cases: (i) \( \mu_{\uparrow, \downarrow} < \eta \), which is equivalent to the situation where \( T = \mu_{\uparrow, \downarrow} = 0 \) studied in section 3.2, and (ii) \( \mu_{\uparrow, \downarrow} > \eta \). For \( \mu_{\uparrow, \downarrow} > \eta \) we have

\[
[y(\eta, \mu_{\uparrow, \downarrow}) + G(\eta, \mu_{\uparrow, \downarrow})] \left[ \eta - \Delta + \frac{\lambda_{GN}}{2\pi N} \eta y(\eta, \mu_{\uparrow, \downarrow}) \right] - \frac{\lambda_{GN}}{2\pi N} \eta = 0,
\]

where

\[
y(\eta, \mu_{\uparrow, \downarrow}, T = 0) \equiv y(\eta, \mu_{\uparrow, \downarrow}) = \ln \left( \frac{m_F}{\eta} \right) - \frac{1}{2} \ln \left( \frac{\mu_1 + \sqrt{\mu_1^2 - \eta^2}}{\eta} \right) + \ln \left( \frac{\mu_1 + \sqrt{\mu_1^2 - \eta^2}}{\eta} \right),
\]

(3.77)

and we have defined the function

\[
G(\eta, \mu_{\uparrow, \downarrow}) \equiv G = \frac{1}{2} \left( \frac{\mu_1}{\sqrt{\mu_1^2 - \eta^2}} + \frac{\mu_1}{\sqrt{\mu_1^2 - \eta^2}} \right) - 1.
\]

(3.78)

Using

\[
y(\eta, \mu_{\uparrow, \downarrow}) = \frac{\pi \Delta}{\lambda_{GN} \eta},
\]

(3.79)

from \( \frac{d\mathcal{F}}{d\Delta} = 0 \) in equation (3.76), we find a second-order equation for \( \Delta \):

\[
\frac{\pi}{\lambda_{GN} \eta} \left( 1 - \frac{1}{2N} \right) \Delta^2 - \left[ \frac{\pi}{\lambda_{GN}} - G \left( 1 - \frac{1}{2N} \right) \right] \Delta - \left( G - \frac{\lambda_{GN}}{2\pi N} \right) \bar{\eta} = 0,
\]

(3.80)

whose solution is

\[
\Delta = \frac{1}{2} \left( 1 - \frac{1}{2N} \right) \left\{ 1 - \frac{\lambda_{GN}}{\pi} \left( 1 - \frac{1}{2N} \right) G + \sqrt{\left[ 1 + \frac{\lambda_{GN}}{\pi} \left( 1 - \frac{1}{2N} \right) G \right]^2 - \frac{2}{N} \left( 1 - \frac{1}{2N} \right) \left( \frac{\lambda_{GN}}{\pi} \right)^2} \right\}.
\]

(3.81)

We have taken the positive solution from equation (3.80) since the limit \( \lambda \to 0 \) of equation (3.81) correctly reproduces the solution of first order in \( \delta \) displayed in equation (3.70). The equation above can be easily expanded in powers of the coupling constant \( \lambda_{GN} \):

\[
\Delta \simeq \frac{\bar{\eta}}{\left( 1 - \frac{1}{2N} \right)} \left\{ 1 - \frac{1}{2N} \left( 1 - \frac{1}{2N} \right) \left( \frac{\lambda_{GN}}{\pi} \right)^2 \right. + \left. \frac{1}{2N} \left( 1 - \frac{1}{2N} \right)^2 \left( \frac{\lambda_{GN}}{\pi} \right)^3 G + \vartheta \left( \frac{\lambda_{GN}}{\pi} \right)^4 \right\}.
\]

(3.82)
We can plug $\Delta$ from equation (3.79) into equation (3.82) and obtain an equation for $\bar{\eta}$ which, for small values of $(\lambda_{GN}/\pi)$, reads

$$Y(\eta, \mu_{\uparrow}, \mu_{\downarrow}) = \frac{\pi}{\lambda_{GN}} \left( 1 - \frac{1}{2N} \right),$$

where $Y$ is given by equation (3.77). The equation above cannot be solved in a closed form for $\bar{\eta}$ as a function of $\mu_{\uparrow}$, $\mu_{\downarrow}$. However, for $\delta \mu = 0$, i.e., for $\mu_{\uparrow} = \mu_{\downarrow} = \mu$, it can be easily solved and generalizes equation (3.71) for non-zero values of the chemical potential, yielding

$$\bar{\eta}_{\delta_1}(\mu) = \sqrt{\bar{\eta}_{\delta_1}(0)(2\mu - \bar{\eta}_{\delta_1}(0))},$$

where $\bar{\eta}_{\delta_1}(0)$ is given by equation (3.71), and $(\bar{\eta}_{\delta_1}(0)/2) \leq \mu \leq \bar{\eta}_{\delta_1}(0)$. With this equation we find to this order

$$\Delta_{\delta_1}(\mu) = \left( 1 - \frac{1}{2N} \right)^{-1} \bar{\eta}_{\delta_1}(\mu).$$

As for $\Delta_{\delta}(0)$ given by equations (3.72), (3.85) obtained from the OPT approach explicitly includes corrections beyond large $N$ to the mean-field result. Note that the equation above is reduced to the mean-field (local maximum) result, given by equation (3.9), in the limit $N \to \infty$, as it should be.

3.3.4. The number densities at zero temperature beyond the mean-field level. As we have seen before, the densities are obtained from the usual relation $n_{\uparrow,\downarrow} = -\partial/\partial \mu_{\uparrow,\downarrow} V_{\text{eff}}(T, \mu_{\uparrow,\downarrow}, \Delta)$ at $\Delta = \Delta_{\text{min}} \equiv \bar{\Delta}$. Now since we are considering corrections to the large $N$ results, we have to include the other minimum condition $\eta = \bar{\eta}$. Then we want to know how the corrections beyond the mean-field level will affect the densities given by equation (3.34). Then one obtains

$$n_{\uparrow,\downarrow}(T, \mu_{\uparrow}, \mu_{\downarrow}) = \frac{1}{\varepsilon_F h} \left[ \left( kT \right)^2 N I_1(\eta, \mu_{\uparrow,\downarrow}, T) + \eta(\eta - \Delta) \right] \frac{N}{2\pi} I_2(\eta, \mu_{\uparrow,\downarrow}, T) + \frac{\lambda_{GN}}{4\pi^2} \eta^2 \frac{\pi}{2} \left[ \left( kT \right)^2 I_3(\eta, \mu_{\uparrow,\downarrow}, T) I_3'(\eta, \mu_{\uparrow,\downarrow}, T) \right] \right|_{\eta=\bar{\eta}, \Delta=\bar{\Delta}},$$

where the primes indicate derivatives with respect to $\mu_{\uparrow,\downarrow}$.

Since in this subsection we are interested in obtaining the zero-temperature corrections to the densities beyond the mean-field level, the thermal effects will be neglected.

Using equations (3.73)–(3.75) in Landau’s free energy density, equation (3.62), we observe that it can again be divided into two cases: (i) $\mu_{\uparrow,\downarrow} < \eta$ and (ii) $\mu_{\uparrow,\downarrow} > \eta$. The case $\mu_{\uparrow,\downarrow} < \eta$ is equivalent to the situation where $T = \mu_{\uparrow,\downarrow} = 0$ giving $n_{\uparrow,\downarrow}(T = 0, \mu_{\uparrow} < \eta, \mu_{\downarrow} < \eta) = 0$. For case (ii) one has to resort to the numerical solution of the nonlinear equations above.
4. The massive Gross–Neveu model and cis-polyacetylene

4.1. The MGN model Lagrangian

The cis-polyacetylene form has non-degenerate ground states and is appropriately described by the massive Gross–Neveu model (MGN) model. The MGN model is obtained when the discrete chiral symmetry is explicitly broken by adding to the Lagrangian (2.13) a fermion bare mass term \( M \) for both the spin-\( \uparrow \) and spin-\( \downarrow \) electrons:

\[
\mathcal{L}_{\text{MGN}} = \sum_{j=1,2} \bar{\psi}_j \left[ -\gamma_0 \hbar \partial_x + i \hbar v_F \gamma_1 \partial_x - \Delta(x) - M + \gamma_0 \mu_j \right] \psi_j - \frac{1}{\hbar v_F \lambda_{\text{GN}}} \Delta^2(x). \tag{4.1}
\]

The bare mass term \( M \) corresponds \cite{34} to the Brazovskii and Kirova external contribution from the rigid polymer skeleton to the total gap \cite{13}. As we will see below, the presence of a mass term ensures the elimination of kink–antikink configurations, which are suppressed in the thermodynamical limit even in the presence of finite chemical potentials for the electrons \cite{54}. Then in this section we examine only homogeneous condensates. In the presence of a mass term it is more convenient to redefine the \( \Delta \) field by shifting it by a constant \( \Delta \to \Delta + M \). Then the Lagrangian (apart from constant terms) reads

\[
\mathcal{L}_{\text{MGN}} = \sum_{j=1,2} \bar{\psi}_j \left[ -\gamma_0 \hbar \partial_x + i \hbar v_F \gamma_1 \partial_x - \Delta - \gamma_0 \mu_j \right] \psi_j - \frac{2M}{\hbar v_F \lambda_{\text{GN}}} \Delta - \frac{1}{\hbar v_F \lambda_{\text{GN}}} \Delta^2. \tag{4.2}
\]

4.1.1. The effective potential of the MGN model at zero temperature and zero chemical potential.

Proceeding as before, we obtain the following expression for the renormalized effective potential of the MGN model at zero temperature and chemical potential:

\[
V_{\text{eff}}(\Delta, M) = \frac{\Delta^2}{\hbar v_F} \left( \frac{1}{\lambda_{\text{GN}}} - \frac{3}{2\pi} \right) + \frac{\Delta^2}{\pi \hbar v_F} \ln \left( \frac{\Delta}{m_F} \right) + \frac{2M}{\hbar v_F \lambda_{\text{GN}}} \Delta. \tag{4.3}
\]

Substituting \( m_F \) from the solution for \( \Delta \) when \( M = 0 \) we find

\[
V_{\text{eff}}(\Delta, M) = \frac{\Delta^2}{2\pi \hbar v_F} \left[ \ln \left( \frac{\Delta^2}{\Delta_0^2} \right) - 1 \right] + \frac{2M}{\hbar v_F \lambda_{\text{GN}}} \Delta. \tag{4.4}
\]

The minimization for \( V_{\text{eff}}(\Delta, M) \) gives

\[
\Delta \ln \left( \frac{\Delta^2}{\Delta_0^2} \right) + \frac{2\pi M}{\lambda_{\text{GN}}} = 0. \tag{4.5}
\]

From the equation above it is easy to see that when \( M = 0 \) the solutions are \( \Delta = 0 \) and \( \Delta = \pm \Delta_0 \) at \( x = \pm \infty \), interpolated by a kink, as seen in section 3. Besides, we have that \( V_{\text{eff}}(\Delta = 0) = 0 \) and \( V_{\text{eff}}(\Delta = \pm \Delta_0) = -\Delta_0^2/2\pi \hbar v_F \). Then, since \( \Delta = 0 \) corresponds to a local maximum, the minima are degenerate at \( \pm m_F e^{i\pi/\lambda_{\text{GN}}} \). For any \( M \neq 0 \) we have the disappearance of the degenerate vacuum (minima), as well as the kink, giving place to a unique solution for a given value of \( M \) \cite{55}. As pointed out in \cite{55}, if any soliton exists at all, its stability has to depend on the energetics of trapping fermions.

Equation (4.5) is very sensitive to the value of \( M \). In other words, there will be solutions for (positive) \( \Delta \) only up to a maximum value of \( M \). If we define a dimensionless function \( f(x, \bar{M}) \equiv f(x) = x^2 \ln(x^2) + \bar{M} x \), where \( x \equiv \Delta/\Delta_0 \) and \( \bar{M} \equiv 2\pi M / \lambda_{\text{GN}} \Delta_0 \), we

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have to solve self-consistently \( f(x) = 0 \) and \( f'(x) = df(x)/dx = 0 \) to obtain the windows for \( M \) and \( \Delta_0(M) \):

\[
0 \leq M \leq \frac{\lambda_{GN}\Delta_0}{\pi\epsilon}, \quad \frac{\Delta_0}{\epsilon} \leq \Delta_0(M) \leq \Delta_0. \tag{4.6}
\]

The effect of a mass term in the MGN model can be summarized simply as: as \( M \) is increased from 0 to \( M_{\text{max}} = \lambda_{GN}\Delta_0/\pi\epsilon \), the minimum of \( V_{\text{eff}}(\Delta, M) \) moves smoothly from \( \Delta_0 \) to \( \Delta_0/\epsilon \).

4.1.2. The effective potential of the MGN model at zero temperature and finite chemical potential.

Since after the change of variable \( \Delta \to \Delta + M \) the mass parameter \( M \) enters only in the classical part of the effective potential, it can be written as

\[
V_{\text{eff}}(\Delta, M, \mu_{\uparrow}, \mu_{\downarrow}) = V_{\text{eff}}(\Delta, M) + \Theta_1 F_1 + \Theta_2 F_2, \tag{4.7}
\]

where \( V_{\text{eff}}(\Delta, M) \) is given by equation (4.4) and \( F_1,2 \) are defined after equation (3.7). The extremization of \( V_{\text{eff}}(\Delta, M, \mu_{\uparrow,\downarrow}) \) yields

\[
\Delta \left[ \ln \left( \frac{\Delta^2}{\Delta_0^2} \right) + \Theta_1 G_1 + \Theta_2 G_2 \right] + \frac{2\pi M}{\lambda_{GN}} = 0, \tag{4.8}
\]

where \( G_1,2 \equiv \ln((\mu_{\uparrow,\downarrow} + \sqrt{\mu_{\uparrow,\downarrow}^2 - \Delta^2})/\Delta) \). In the limit \( M \to 0 \), equation (4.8) reduces to equation (3.8). The equation above can be solved only numerically for arbitrary values of \( \mu_{\uparrow,\downarrow} \) and \( M \). However, for \( \delta \mu = 0 \) we obtain the following \( \mu \) and \( M \) dependent equation to first order in \( M/\Delta \):

\[
\Delta^3 + (\Delta_0^2 - 2\Delta_0\mu)\Delta - \frac{2\pi M}{\lambda_{GN}}(\Delta_0 - \mu)\Delta_0 = 0. \tag{4.9}
\]

This equation has analytical solutions:

1. When \( \mu = \Delta_0/2 \), \( \Delta = \Delta_0(\pi M/\lambda_{GN}\Delta_0)^{1/3} \).
2. When \( \mu = \Delta_0 \), \( \Delta = 0 \). The other solution, \( \Delta = \Delta_0 \), is a local maximum. This can be understood simply as: for small \( M \) and such a large value of \( \mu \) the broken symmetry has been restored.

For other values of \( \mu \), equation (4.9) has to be solved numerically.

5. Summary of the results

We show in table 1 several physical quantities calculated within the GN model for mean-field and OPT (beyond mean-field) approximations under various medium conditions, i.e., temperatures and densities. The places in the table marked with ? indicate that, to the best of our knowledge, there are no studies concerning that physical quantity at mean-field level and beyond in that situation.

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### 6. Conclusions

We have studied the influence of an external Zeeman magnetic field $B_0$ on 1D (CH)$_x$ chains, which can be converted into a partially or fully polarized organic conductor, depending on the intensity of the $B_0$ applied on the wire. The mean-field finite temperature phase diagram of the chain has been investigated. We found that the gap parameter and the magnetization (as well as the densities and density imbalance, and the magnetic susceptibility) of this 1D material under $B_0$ have a similar second-order behaviors until their respective tricritical points are reached. Below these points the transitions are of first order. We found these two tricritical points analytically.

We have shown that the location of the tricritical point in the $t (= T/T_c(0))$ versus $\nu (=(7\xi(3)/8\pi^2)(\mu_1^2+\mu_2^2)/(k_BT_c(0))^2)$ phase diagram stays at the same place by considering both homogeneous and inhomogeneous condensates, such as occur in symmetric $\delta\mu = B_0 = 0$ systems [33–36]. We have found the critical magnetic field $B_{0,c}$ necessary for having a fully polarized organic conductor at zero and finite temperature. We found that for a given magnetic field below $B_{0,c}$, partial polarizations (magnetizations) can be realized experimentally, provided that the temperatures are kept outside the ‘non-metallic’ region of figure 2. It is worth noting that, according to equation (3.42), for other 1D systems with a smaller critical chemical potential or with a greater effective $g$-factor, a smaller critical magnetic field necessary for a full polarization of these 1D chains would be found.

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**Table 1.** Physical quantities calculated using approximations at MF level and beyond and in various situations for the temperature and chemical potentials. The inhomogeneous gap parameter at zero $T$ and finite $\mu$ marked with the * symbol is discussed below equation (3.51). $\Delta_0(\varsigma)$ is given by equation (3.52).

| Approximation                              | Homogeneous | Inhomogeneous |
|--------------------------------------------|-------------|---------------|
| MF at zero $\mu$ and zero $T$             | $\Delta_0 = m_F e^{1-\pi/\lambda GN}$ | $\Delta_0\tanh(\Delta_0 x)$ |
| MF at finite $\mu$ and zero $T$           | $\Theta(\mu_c - \mu)\Delta_0$ * | 0 |
| MF at finite $\mu_{\uparrow,\downarrow}$ and zero $T$ | Num. solut. of equation (3.8) | ? |
| MF at finite $\mu_{\uparrow,\downarrow}$ and high $T$ | $\sqrt{-\frac{\alpha_2}{2\alpha_4}} \Delta_0(\varsigma) \sqrt{\varsigma} \text{sn}(\Delta_0 x; \varsigma)$ | Equation (3.43) |
| Beyond MF at zero $T$ and zero $\mu$      | $F(N)^{-1} m_F e^{-\pi/\lambda GN} F(N)$ | ? |
| Beyond MF at finite $\mu_{\uparrow,\downarrow}$ and zero $T$ | Num. solut. of equation (3.83) | ? |
| Beyond MF at finite $\mu_{\uparrow,\downarrow}$ and $T$ | ? | ? |

$\Delta_0(\varsigma)$ is given by equation (3.52), $F(N) = 1 - 1/2N$, $M$ is the Pauli magnetization and $\chi$ is the magnetic susceptibility—which are, of course, zero for $\delta\mu = (g/2)\mu_B B_0 = 0$.
In table 1 we show the homogeneous and inhomogeneous gap parameter $\Delta(x)$, the Pauli magnetization $M$ and the magnetic susceptibility $\chi$, and zero and finite $T$ and $\mu$ calculated at mean-field approximation level and beyond. For the quantities identified with $\ast$, further investigations are needed to find them.

We have also seen that the consideration of electron correlations in the investigation of some specific properties of 1D CH chains is of crucial importance. We intend to analyze a continuum version of the Hamiltonian of equation (2.6) within the quantum field theory approach, and publish this elsewhere.

A direct extension of the present work would be the investigation of the possibility of using polymers or graphene ribbons as spin-polarized conductors, upon the joint application of a Zeeman and an electric field in the system. This would enable us to study the transport properties of 1D chains at zero and finite temperature.

As a next step in the investigation of the effects of magnetic fields on 1D systems, we would like to study the results of parallel and perpendicular magnetic fields applied simultaneously and independently on a polymer or graphene wire. This could open up interesting possibilities for using such materials in practical applications as electronic devices.

The methods we used here, based on the calculation of the (grand) effective potential free energy, which are more suitable for the analysis of the phase structure of the model, are useful also for the study of the consequences of a perpendicular magnetic field applied in the system. Indeed, one can incorporate the effects of a magnetic background on the effective potential and investigate how the chiral transition and the condensate (in our case the $\Delta$ gap) are modified. Assuming that the system is now in the presence of a strong magnetic field background that is constant and homogeneous, one can compute the modified effective potential following the procedure presented in detail in [56]–[59].

We hope to make further studies on the magnetic properties of these systems based on the model we have studied here, and to report on them in the future.

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