Variational description of the dimensional cross-over in the array of coupled one-dimensional conductors

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Abstract

Variational wave function is proposed to describe electronic properties of an array of one-dimensional conductors coupled by transverse hopping and interaction. For weak or intermediate in-chain interaction the wave function has the following structure: Tomonaga-Luttinger bosons with momentum higher than some variational quantity $\tilde{\Lambda}$ are in their ground state while other bosons (with $|k| < \tilde{\Lambda}$) form kinks – fermion-like excitations of the Tomonaga-Luttinger boson field. Nature of the ground state for this quasiparticles can be determined by solving three dimensional effective hamiltonian. Since the anisotropy of the effective hamiltonian is small the use of the mean field theory is justified. For repulsive interaction possible phases are density wave and $p$-wave superconductivity. Our method allows us to calculate the low-energy part of different electronic Green’s functions. In order to do that it is enough to apply standard perturbation theory technique to the effective hamiltonian. When the in-chain interaction is strong $\tilde{\Lambda}$ vanishes and no fermionic excitation is present in the system. In this regime the dynamics is described by transversally coupled Tomonaga-Luttinger bosons.
I. INTRODUCTION

The adequate description of quasi-one-dimensional (Q1D) conductors remains an unresolved theoretical challenge. Experimentally, at low temperature such systems either three dimensional anisotropic Fermi liquids or they freeze into a three dimensional phase with broken symmetry\[1\]. At high temperature their transport properties show many unusual features generally attributed to the one-dimensional electron anisotropy. This cross-over from 1D to 3D is the core problem of Q1D physics.

It is possible to look at the issue of the dimensional cross-over from another angle. At high temperature the proper elementary excitations of the system are Tomonaga-Luttinger (TL) bosons. When the temperature is low and the interaction is weak enough the elementary excitations are fermions. Therefore, to describe the system at different energy scales one needs to explain how high-energy bosons ‘cross over’ into low-energy fermions. Obviously, this is a non-trivial task.

In this paper we develop a variational approach which accomplishes this goal. To explain the structure of the variational wave function let us first consider a one-dimensional conductor described by TL hamiltonian. The ground state of this system is the ground state of TL bosons with all momenta $k$. Let’s turn the transverse hopping on and couple $N_\perp$ of these conductors into 3D array. In this situation the system will attempt to lower its ground state energy even further by taking advantage of the transverse hopping energy. However, in order to participate in hopping the bosons have to form many-body fermion-like excitations which have finite overlap with the physical fermion.

To accommodate for possibility of having two types of excitations, bosonic and fermionic, we device our variational state in the following fashion. We introduce intermediate cut-off $\tilde{\Lambda} < \Lambda$, where $\Lambda$ is the cut-off of the 1D hamiltonian. All TL bosons whose energy and momenta are high ($|k| > \tilde{\Lambda}$) remain in their ground states. The small momenta bosons ($|k| < \tilde{\Lambda}$) form fermion-like excitations which are delocalized in transverse direction. To distinguish between the physical electrons and these fermionic excitations we will refer to the latter as quasiparticles. In other words, the wave function can be factorized into two parts. High-energy part corresponds to the ground state of $|k| > \tilde{\Lambda}$ TL bosons, low-energy
part corresponds to the 3D anisotropic Fermi liquid composed of the quasiparticles.

The variational energy is minimized by adjusting $\tilde{\Lambda}$. The energy of quasiparticle transverse hopping is decreasing function of $\tilde{\Lambda}$. At the same time, the in-chain energy grows when $\tilde{\Lambda}$ grows. The trade-off between the transverse kinetic energy and the in-chain potential energy determines the value of $\tilde{\Lambda}$.

If the optimal value of $\tilde{\Lambda}$ is non-zero the low-energy excitations of the system are the quasiparticles. Properties of the fermionic quasiparticle state depend on quasiparticle effective hamiltonian. It arises naturally after high-energy bosons are ‘integrated out’. In this effective hamiltonian the anisotropy is insignificant. Standard many-body techniques such as perturbation theory and mean field theory can be used to calculate Green’s functions and map out the quasiparticle phase diagram. Since the physical electron and the quasiparticle have finite overlap there is a direct correspondence between the broken symmetry phases of the effective hamiltonian and the physical system. We will show that possible phases for spinless Q1D electrons with repulsion are the charge density wave (CDW) and the superconductivity with the Cooper pairs formed of the electrons on neighboring 1D chains.

As the in-chain interaction grows parameter $\tilde{\Lambda}$ approaches zero. When $\tilde{\Lambda}$ vanish the fermionic excitations cease to exist. The system is described by 3D TL boson state. In such a regime the ground state is CDW.

Our approach allows us to obtain some new analytical results. With the help of the method it is possible to derive a formula for quasiparticle damping near Fermi surface. Also, we evaluate transition temperatures for CDW and superconductivity. The knowledge of these temperatures allows us to map out the phase diagram of our system. Although, these quantities have been obtained using different numerical techniques [2, 3] the analytical expressions had not been reported.

The paper is organized as follows. In Section II we determine $\tilde{\Lambda}$ and derive the effective hamiltonian for the fermions. Section III contains the evaluation of the single-particle Green’s function. Different phases of the effective hamiltonian (and the physical system) are mapped in Section IV. The regime where $\tilde{\Lambda} = 0$ is discussed in Section V. We give our conclusions in Section VI.
II. VARIATIONAL PROCEDURE

We start our analysis by writing down the hamiltonian for the array of coupled 1D conductors:

\[ H = \int_0^L dx H, \]
\[ \mathcal{H} = \sum_i \mathcal{H}_i^{1d} + \sum_{i,j} \mathcal{H}_{ij}^{1d}, \]
\[ \mathcal{H}_i^{1d} = i v_F \left( \psi_{Li}^\dagger \nabla \psi_{Li} - \psi_{Ri}^\dagger \nabla \psi_{Ri} \right) + g \psi_{Li}^\dagger \psi_{Li} \psi_{Ri}^\dagger \psi_{Ri}, \]
\[ \mathcal{H}_{ij}^{1d} = -t(i-j) \sum_{p=L,R} \left( \psi_{pi}^\dagger \psi_{pj} + \text{h.c.} \right) + g_{2k_F}(i-j) \left( \psi_{Li}^\dagger \psi_{Ri}^\dagger \psi_{Lj} \psi_{Rj} + \text{h.c.} \right) \]
\[ + g_0(i-j) \left( \psi_{Li}^\dagger \psi_{Li} + \psi_{Ri}^\dagger \psi_{Ri} \right) \left( \psi_{Lj}^\dagger \psi_{Lj} + \psi_{Rj}^\dagger \psi_{Rj} \right), \]

with the real-space cut-off \( a = \pi/\Lambda \). The fermionic field \( \psi_{pi}^\dagger \) creates physical electron with the chirality \( p = L(+) \) or \( p = R(-) \) on chain \( i \). Transverse interaction constants \( g_0 \) (forward scattering) and \( g_{2k_F} \) (exchange) are positive. The terms proportional to \( g_0 \) and \( g_{2k_F} \) account for the Coulomb repulsion of the electrons on different chains. It is further assumed that:

\[ g > g_0 > g_{2k_F}. \]

Now we use Abelian bosonization prescription [4]:

\[ \psi_p^\dagger(x) = (2\pi a)^{-1/2} \eta_p e^{i\sqrt{2\pi} \varphi_p(x)} = (2\pi a)^{-1/2} \eta_p e^{i\sqrt{\pi} (\Theta(x) + \text{p}\Phi(x))}, \]

(6)

to express the electron hamiltonian in terms of bosonic fields. In the above formula \( \eta_p \) are Klein factors, \( \Theta \) is the TL boson field, \( \Phi \) is the dual field. The bosonized one-chain hamiltonian is:

\[ \mathcal{H}_{1d}^{1d} [\Theta, \Phi] = \frac{v_F^2}{2} \left( : (\nabla \Theta)^2 : + : (\nabla \Phi)^2 : \right) + \frac{g}{4\pi} \left( : (\nabla \Phi)^2 : - : (\nabla \Theta)^2 : \right). \]

(7)

The symbol : \ldots : denotes normal ordering of TL boson operators with respect to non-interacting \((g = 0)\) ground state.

Let us introduce our main variational parameter \( \tilde{\Lambda} < \Lambda \) and use it to split TL boson fields into fast \((\Lambda > | |k|| - k_F| > \tilde{\Lambda}, \text{subscript ‘>’})\) and slow \((| |k|| - k_F| < \tilde{\Lambda}, \text{subscript ‘<’})\) modes:

\[ \mathcal{H}_{1d}^{1d} [\Theta, \Phi] = \mathcal{H}_{<}^{1d} + \mathcal{H}_{>}^{1d} = \mathcal{H}_{<}^{1d} [\Theta_<, \Phi_<] + \mathcal{H}_{>}^{1d} [\Theta_>, \Phi_>] \].

(8)
We define the fermionic field $\Psi_p^\dagger(x)$ with the help of equation (6) in which $a$ is substituted by $\tilde{a} = \pi/\Lambda$ and $\Theta_<$ and $\Phi_<$ are placed instead of $\Theta$ and $\Phi$. The field $\Psi$ is our quasiparticle discussed in Introduction. Using this field we re-fermionize $H_{ij}^{1d}$. The result is the same as (3) with $\Psi_p$ instead of $\psi_p$. The transverse terms (4) can be easily re-written if one observe that the physical fermion is simply:

$$\psi_p^\dagger = \sqrt{\tilde{a}/a} \Psi_p^\dagger e^{i\sqrt{\pi}(\Theta_+ + \Phi_+)},$$

and that the fermionic and bosonic parts in this definition commute with each other. Therefore, $H_{ij}^{1d}$ is equal to

$$H_{ij}^{1d} = - (\tilde{a}/a) t(i - j) \sum_{p=L,R} \left( \Psi_p^\dagger \Psi_{p,j} e^{i\sqrt{\pi}((\Theta_+ - \Theta_+) + p(\Phi_+ - \Phi_+))} + \text{h.c.} \right)$$

$$+ \tilde{a}/a^2 g_{2k}(i - j) \left( \Psi_{L,i} \Psi_{R,j}^{\dagger} \Psi_{L,j} \Psi_{R,i}^{\dagger} e^{i\sqrt{\pi}(\Phi_+ - \Phi_+)} + \text{h.c.} \right)$$

$$+ g_0(i - j) \left( \left( \Psi_{L,i}^{\dagger} \Psi_{R,i} + \Psi_{R,i}^{\dagger} \Psi_{L,i} \right) \left( \Psi_{L,j}^{\dagger} \Psi_{L,j} + \Psi_{R,j}^{\dagger} \Psi_{R,j} \right) + \frac{1}{\pi} \nabla \Phi_+ \nabla \Phi_+ \right).$$

Our variational wave function has the form:

$$|\text{Var}\rangle = |\{\Psi_{pi}\}\rangle \prod_j \langle 0_{j>} | \prod_j (2|k|/\pi K)^{1/2} \exp \left\{ -|k| |\Phi_{jk}|^2 / K \right\}. \quad (11)$$

It is a product of some many-body state $|\{\Psi_{pi}\}\rangle$ composed of the quasiparticles $\Psi_{pi}$ and the ground states $|0_{j>}\rangle$ of $H^{1d}[\Theta_+, \Phi_+]$.

Variational ground state energy is found by minimizing the expression:

$$E^V = N L \frac{\theta u}{4\pi} \left( \Lambda^2 - \Lambda^2 \right) + \langle \{\Psi_{pi}\}\rangle \left( \int_0^L dx H^\text{eff} \right) |\{\Psi_{pi}\}\rangle, \quad (12)$$

$$H^\text{eff} = \sum_i i v_F \left( \Psi_{Li}^\dagger \partial_x \Psi_{Li} - \Psi_{Li}^\dagger \partial_x \Psi_{Li} \right) + g \Psi_{Li}^\dagger \Psi_{Li} \Psi_{Li}^\dagger \Psi_{Li}$$

$$- \sum_{ij} \sum_{p=L,R} \tilde{t}(i - j) \left( \Psi_{pi}^\dagger \Psi_{pj} + \text{h.c.} \right) + \sum_{ij} \tilde{g}_{2k}(i - j) \left( \Psi_{Li}^\dagger \Psi_{Ri} \Psi_{Lj}^\dagger \Psi_{Rj} + \text{h.c.} \right)$$

$$+ g_0(i - j) \left( \Psi_{Li}^\dagger \Psi_{Li} + \Psi_{Ri}^\dagger \Psi_{Ri} \right) \left( \Psi_{Li}^\dagger \Psi_{Lj} + \Psi_{Rj}^\dagger \Psi_{Rj} \right),$$

$$\tilde{t} = \zeta^\theta \tilde{t}, \quad \tilde{g}_{2k} = \zeta^{2\kappa - 2} g_{2k}, \quad \zeta = \tilde{\Lambda}/\Lambda. \quad (14)$$

The number of chains is $N_\perp$. The TL liquid parameter $\kappa$, the electron anomalous dimension $\theta$ and boson velocity $u$ are defined in the usual way:

$$\kappa = \sqrt{\frac{2\pi v_F - g}{2\pi v_F + g}}, \quad \theta = \frac{1}{2} \left( \kappa + \kappa^{-1} - 2 \right), \quad u = \frac{1}{2\pi} \sqrt{(2\pi v_F - g)(2\pi v_F + g)}.$$

(15)
The first term of (12) has purely one-dimensional origin. The second term is the energy of the quasiparticle ground state.

Observe that the parameters of the effective hamiltonian \( \tilde{t}/\tilde{\Lambda} \) and \( \tilde{g}_{2k_F} \) are connected to the corresponding bare parameters as if they are subject to the renormalization group (RG) flow in the vicinity of the TL fixed point. The explanation to this fact is quite obvious: our method of deriving the effective hamiltonian is equivalent to the tree level RG scaling near TL fixed point.

If the transversal interactions are small (\( g_0 \) and \( \tilde{g}_{2k_F} \) both less then \( \tilde{t}/\tilde{\Lambda} \)) they can be neglected. In addition, we neglect corrections to the energy due to spontaneous symmetry breaking. The latter assumption works when \( \theta \ll 1 \). Its validity away from this point will be discussed at the end of Section V. Under these two conditions the expression (12) becomes:

\[
E^V/(LN_\perp) \approx \frac{\theta u}{4\pi} \left( \zeta^2 - 1 \right) \Lambda^2 - \frac{2}{\pi v_F} \zeta^{2\theta} \sum_i (t(i))^2. 
\] (16)

This variational energy attains its minimum at

\[
\zeta = \begin{cases} 
(8\tilde{t}^2/uv_F\Lambda^2)^{1/(2-2\theta)} & \text{if } \theta < 1, \\
0 & \text{if } \theta > 1,
\end{cases}
\] (17)

\[
\tilde{t}^2 = \sum_i (t(i))^2. 
\] (18)

We have to remember, however, that value of the numerical coefficient in (17) is not accurate. This is due to the fact that the second term in (16) is calculated under assumption \( \tilde{t} < \tilde{\Lambda} \). When \( \tilde{\Lambda} \) gets smaller the coefficient in front of this term acquires some \( \tilde{\Lambda} \) dependence. We neglect the corrections due to this dependence since they are less singular (at small \( \tilde{\Lambda} \)) then the second term of (16). These corrections modify the result for \( \zeta \) quantitatively, therefore, it is more appropriate to write

\[
\zeta \propto \left( \frac{t}{u\Lambda} \right)^{1/(1-\theta)}, 
\] (19)

\[
\bar{u} = \sqrt{uv_F}. 
\] (20)

Using this formula it is easy to show that:

\[
\tilde{t} \propto \bar{u}\tilde{\Lambda} \propto t \left( \frac{t}{u\Lambda} \right)^{\theta/(1-\theta)}. 
\] (21)

This means that for \( \theta < 1 \) the effective transverse hopping amplitude \( \tilde{t} \) of the quasiparticle \( \Psi \) is of the same order as the quasiparticle longitudinal cut-off energy \( v_F\tilde{\Lambda} \). Therefore, due
to small anisotropy, the Hamiltonian for the quasiparticles (13) can be treated within the framework of usual mean field theory and perturbation theory.

Our calculations, in agreement with renormalization group analysis [5, 6], show that for $\theta < 1$ there is the cross-over energy scale $\tilde{t}$ above which the system is equivalent to a collection of decoupled chains while below the transverse hopping becomes important.

Depending on the interaction and the anisotropy the region $\theta < 1$ can be further split into two parts. The transverse hopping contribution to the variational energy (second term of (16)) can be re-written as follows:

$$\frac{2}{\pi v_F} t^2 \propto \frac{2}{\pi v_F} t^2 \exp \left( -\frac{2\theta}{1-\theta} \log \left( \frac{\bar{u}\Lambda}{t} \right) \right).$$

If the argument of the exponential function is small the exponential can be replaced by the first few terms of the Taylor series. In such a situation the contribution of the in-chain interaction to the total energy, eq. (16), can be calculated perturbatively. One-dimensional effects are virtually unobservable. This is the weak coupling regime.

When the anisotropy and the in-chain interaction are strong the exponential cannot be approximated accurately by the low order Taylor expansion. The system is in the intermediate coupling regime now. In order to obtain a reliable answer in such a regime it is not enough to apply finite-order perturbation theory. Our method converts the system of physical electrons with intermediate coupling into the system of quasiparticles with weak coupling. The latter can be studied by standard perturbation theory.

As a function of the bare transverse hopping amplitude $t$ the cross-over from the weak coupling to the intermediate coupling occurs at:

$$t^* \propto \bar{u}\Lambda \exp \left( -\frac{1-\theta}{\theta} \right).$$

For the weak in-chain interaction $\theta \ll 1$. If this is the case it is necessary to have exponentially small transverse hopping amplitude $t$ in order to observe non-trivial Q1D effects.

When $\theta > 1$ the effective cut-off momentum $\tilde{\Lambda}$ is zero. The quasiparticles are not formed. The system can be viewed as a collection of TL bosons weakly coupled by the transverse exchange interaction. The possibility of such state was first pointed out by Wen [7]. It is natural to call such a regime strong coupling. Section V is reserved for discussion of strong coupling.
III. SINGLE-ELECTRON GREEN'S FUNCTION

The calculation of different propagators for Q1D system is an open question. Our
approach allows for easy evaluation of the low-energy part of Green’s functions in the in-
termediate coupling regime. The high-energy parts of Q1D Green’s functions are believed to
coincide with the Green’s functions of TL model. The latter have been discussed extensively
in the literature.

The Matsubara propagator of the physical electronic field $\psi_L$ is equal to:

$$G_L(x, R_\perp, \tau) = \frac{1}{\zeta} \langle \mathcal{T} \left\{ \Psi_L^\dagger(x, \tau) \Psi_{Lj}^\dagger(0, 0) \right\} \rangle \times$$

$$\langle \mathcal{T} \left\{ e^{-i\sqrt{\pi}(\Theta_{>i}(x, \tau)+\Phi_{>i}(x, \tau))} e^{i\sqrt{\pi}(\Theta_{>j}(0, 0)+\Phi_{>j}(0, 0))} \right\} \rangle,$$

$$R_\perp = R_i - R_j. \quad (25)$$

The notation $\langle \ldots \rangle_\Psi$ stands for averaging with respect to the quasiparticle ground state $|0_\Psi\rangle$. Likewise, $\langle \ldots \rangle_>$ stands for the expectation value with respect to $|0_>\rangle$ state.

The bosonic part of this formula can be immediately calculated:

$$\frac{1}{\zeta} \langle \mathcal{T} \left\{ e^{-i\sqrt{\pi}(\Theta_{>i}(x, \tau)+\Phi_{>i}(x, \tau))} e^{i\sqrt{\pi}(\Theta_{>j}(0, 0)+\Phi_{>j}(0, 0))} \right\} \rangle_> = \left( \frac{G_{1d}^{Ld}}{\bar{G}_{1d}^{Ld}} \right) \delta_{ij} + \zeta^\theta (1 - \delta_{ij}). \quad (26)$$

Here $G_{1d}^{Ld}$ ($\bar{G}_{1d}^{Ld}$) is the Matsubara Green’s function of the Tomonaga-Luttinger model with the cut-off $\Lambda$ ($\bar{\Lambda}$).

Our variational wave function does not take into account correlations between $\Phi_{>i}(\Theta_{>i})$ and $\Phi_{>j}(\Theta_{>j})$ if $i \neq j$. However, the above formula is correct at least for large $\tau > 1/\bar{u} \bar{\Lambda}$ or small frequency $\omega < u \bar{\Lambda}$ where those correlations are not important. In such a limit the boson part of (24) is a constant equal to $\zeta^\theta$.

Once the bosonic propagator is found it is necessary to calculate the quasiparticle Green’s
function. This can be done with the help of standard diagrammatic technique. If we neglect
interactions between the quasiparticles the single-electron Green’s function is equal to:

$$G_L(i\omega, p_\parallel, p) = \frac{\zeta^\theta}{i\omega + v_F p_\parallel - \tilde{\varepsilon}_p}, \quad (27)$$

where the renormalized transverse kinetic energy is given by:

$$\tilde{\varepsilon}_p = -2\zeta^\theta \sum_i t(i) \cos (p \cdot R_i). \quad (28)$$

This result coincides with the Green’s function derived by RG [2, 6].
Our method allows to improve the above formula for the single-electron propagator by taking interaction between the quasiparticles into account. Neglecting (i) symmetry-breaking which becomes important for very small frequency only and (ii) the transverse couplings $g_0$ and $\tilde{g}_{2kF}$ (see (5)) one can identify three second-order diagrams contributing to the single-quasiparticle self-energy (fig.1). They are: (a) scattering on the polarization bubble of the same chirality as the incoming quasiparticle, (b) scattering on the polarization bubble of the opposite chirality and (c) the vertex correction. The diagrams (a) and (c) are identical in magnitude and opposite in sign. Thus, (b) is the only diagram on fig.1 which needs to be evaluated.

First, we calculate the quasiparticle polarization bubble $\mathcal{P}_R$. It equals to:

$$
\mathcal{P}_R \left( i\Omega, k_\parallel, k \right) = \int_{q||} \delta \left( v_F q|| + \tilde{\varepsilon}_q \right) \frac{v_F k|| + \tilde{\varepsilon}_{q+k} - \tilde{\varepsilon}_q}{i\Omega - v_F k|| - \tilde{\varepsilon}_{q+k} + \tilde{\varepsilon}_q},
$$

(29)

where the notation $\int_{q||} \ldots = (2\pi)^{-3} b^2 \int dq|| dp^2 q \ldots$ is used. The symbol $b$ denotes the transverse lattice constant. The self-energy is equal to:

$$
\Sigma_L \left( i\omega, p_\parallel, p \right) = -T \sum_\Omega \int_{k||k} \mathcal{G}_L \left( i\omega + i\Omega, p_\parallel + k||, p + k \right) \mathcal{P}_R \left( i\Omega, k_\parallel, k \right).
$$

(30)

After summing over $\Omega$ the following expression for the self-energy is derived:

$$
\Sigma_L = -g^2 \int_{k||k} \int_{q||q} \left( v_F k|| + \tilde{\varepsilon}_{k+q} - \tilde{\varepsilon}_q \right) \delta \left( v_F q|| + \tilde{\varepsilon}_q \right) \times
$$

(31)

$$
\frac{n_F \left( v_F k|| + \tilde{\varepsilon}_{k+q} + \tilde{\varepsilon}_q \right) - n_F \left( v_F \left( k_\parallel + p|| \right) + \tilde{\varepsilon}_{k+p} \right)}{i\omega + 2v_F k|| + v_F p|| - \tilde{\varepsilon}_q + \tilde{\varepsilon}_{k+q} - \tilde{\varepsilon}_{k+p}} +
$$

$$
g^2 \int_{k||k} \int_{q||q} \frac{\sinh \left( \left( v_F k|| + \tilde{\varepsilon}_{k+q} + \tilde{\varepsilon}_q / T \right) \right) \left( i\omega + 2v_F k|| + v_F p|| - \tilde{\varepsilon}_q + \tilde{\varepsilon}_{k+q} - \tilde{\varepsilon}_{k+p} \right)}{(v_F k|| + \tilde{\varepsilon}_{k+q} - \tilde{\varepsilon}_q)^2 \left( v_F q|| + \tilde{\varepsilon}_q \right)}.
$$

When $T = 0$ the first term can be further simplified. The Fermi distribution $n_F$ becomes the step-function. In such a situation it is possible to perform integration over $k||$ and $p||$ exactly. The second integral in the above equation appears due to the relation between the Fermi distribution $n_F$ and the Bose distribution $n_B$: $n_B(\omega) + n_F(\omega) = 1 / \sinh(\omega / T)$. At zero temperature this integral vanishes. In the resultant $T = 0$ expression for $\Sigma_L$ the transverse kinetic energy $\tilde{\varepsilon}_q$ always enter in the combination $\tilde{\varepsilon}_{q+k} + \tilde{\varepsilon}_{k+p} - \tilde{\varepsilon}_q$. Therefore, it is convenient to introduce the quantity:

$$
\nu^\perp(\varepsilon^\perp, p) = \int \frac{d^2 q d^2 k}{(2\pi)^4} b^4 \delta \left( \varepsilon^\perp - \tilde{\varepsilon}_{q+k} - \tilde{\varepsilon}_{k+p} + \tilde{\varepsilon}_q \right).
$$

(32)
With this definition the self-energy can be compactly written as follows:

\[ \Sigma_L \left( i\omega, p_\parallel, p \right) = \frac{g^2}{8\pi v_F} p_\parallel \]

\[ -\frac{g^2}{16\pi v_F^2} \int d\varepsilon^\perp \nu^\perp(\varepsilon^\perp, p) \left( i\omega - v_F p_\parallel - \varepsilon^\perp \right) \log \frac{4\tilde{\Lambda}^2}{\omega^2 + (v_F p_\parallel + \varepsilon^\perp)^2}. \]  

(33)

The Green’s function of the physical electron is equal to \( \zeta^\theta(i\omega + v_F p_\parallel - \tilde{\varepsilon}^\perp - \Sigma_L)^{-1} \). Note, that the logarithmic divergence of the self-energy, a hallmark of the Fermi liquid picture break-down in TL model, is capped in the presence of the transverse hopping. This justifies the use of the perturbation theory.

By doing analytical continuation of (33) it is possible to calculate the retarded self-energy \( \Sigma^\text{ret} \) whose imaginary part is the quasiparticle damping:

\[ \gamma = -\text{Im} \Sigma^\text{ret} = \frac{g^2}{8v_F^2} \nu^\perp(-v_F p_\parallel, p)\omega^2. \]  

(34)

The transverse density of states can be estimated as \( \nu^\perp \propto 1/\tilde{t} \). This gives us \( \gamma \propto (g/v_F)^2\omega^2/\tilde{t}. \) On the mass shell \( \omega = -v_F p_\parallel + \tilde{\varepsilon}_p \) the expression for \( \gamma \) becomes:

\[ \gamma = \frac{g^2}{8} \nu^\perp(-v_F p_F, p) \left( p_\parallel - p_F \right)^2 \propto \frac{g^2}{\tilde{t}} \left( p_\parallel - p_F \right)^2 \]  

(35)

where \( (p_\parallel - p_F) \) is the distance from a given point \( (p_\parallel, p) \) of the Brillouin zone to the Fermi surface \( v_F p_F = \tilde{\varepsilon}_p \) along \( x \) direction.

We need to issue a warning in connection to the accuracy of \( \Sigma_L \). It is not correct to think of (33) as \( \mathcal{O}(g^2) \) expression for the physical electron self-energy. Indeed, the physical electron Green’s function (27) already contains all orders of \( g \) entering though the quasiparticle renormalization \( \zeta^\theta \) and renormalized transverse hopping \( \tilde{\varepsilon} \). It is necessary to remember that our variational approach is uncontrollable approximation. It lacks a small parameter controlling the quality of the results. Therefore, it is not clear how accurate the expression (33) is.

In Ref. [2] the self-energy was evaluated numerically for the system with infinite transverse dimensions. However, those calculations are more complicated technically and do not give analytical answer for the self-energy.

IV. PHASE DIAGRAM

In Section II we derived the low-energy effective hamiltonian for the quasiparticles. Now we will apply the mean field theory to obtain the phase diagram of the effective hamiltonian.
The experimentally observable phase diagram for the physical electrons coincides exactly with that of the quasiparticles. To prove this let us calculate \( \langle \psi_R^\dagger \psi_L \rangle \) for \( T \ll \tilde{u}\tilde{\Lambda} \):

\[
\langle \psi_R^\dagger \psi_L \rangle = \frac{1}{\zeta} \langle \psi_R^\dagger \psi_L \rangle \rangle \langle e^{i\pi(\Theta_{>1}+\Phi_{>1})-i\pi(\Theta_{>1}-\Phi_{>1})} \rangle = \zeta^{-1} \langle \psi_R^\dagger \psi_L \rangle \rangle .
\]

(36)

The physical CDW order parameter is proportional to the CDW expectation value of the quasiparticles. Similar formulas can be obtained for other order parameters. For example, \( \langle \psi_R^\dagger \psi_L^\dagger \rangle = 2 \zeta^{1/2} \langle \psi_R^\dagger \psi_L^\dagger \rangle \rangle \) and \( \langle \psi_R^\dagger \psi_L^\dagger \psi_L^\dagger \psi_R^\dagger \rangle = \zeta^2 \langle \psi_R^\dagger \psi_L^\dagger \psi_L^\dagger \psi_R^\dagger \rangle \rangle \). Therefore, we can determine the phase diagram of (1) by mapping the phases of the Hamiltonian (13).

We consider four order parameters. One is the charge-density wave:

\[
\hat{\rho}_{2kF} = \Psi_R^\dagger \Psi_L
\]

(37)

and there are three types of the superconducting order:

\[
\hat{\Delta}_{\pm ij} = \frac{1}{2} \left( \Psi_R^\dagger \Psi_L^\dagger \pm \Psi_L^\dagger \Psi_R^\dagger \right),
\]

(38)

\[
\hat{\Delta}_{0i} = \Psi_L^\dagger \Psi_R^\dagger.
\]

(39)

The in-chain potential energy can be re-written in terms of \( \hat{\rho} \) and \( \hat{\Delta}_0 \) in the following manner:

\[
g \Psi_L^\dagger \Psi_R^\dagger \Psi_L \Psi_R = -g \hat{\rho}_{2kF} \hat{\rho}_{2kF}^\dagger = g \hat{\Delta}_{0i} \hat{\Delta}_{0i}.
\]

(40)

The exchange interaction can be expressed as:

\[
\tilde{g}_{2kF} \left( \Psi_L^\dagger \Psi_R^\dagger \Psi_R \Psi_L + \text{h.c.} \right) = \tilde{g}_{2kF} \left( \hat{\rho}_{2kF} \hat{\rho}_{2kF}^\dagger + \text{h.c.} \right) = 2 \tilde{g}_{2kF} \left( \hat{\Delta}_{-ij} \hat{\Delta}_{-ij}^\dagger - \hat{\Delta}_{+ij} \hat{\Delta}_{+ij}^\dagger \right).
\]

(41)

Finally, a part of the transverse forward scattering which describes the interaction between the fermions of different chiralities is equal to:

\[
g_0 \left( \Psi_L^\dagger \Psi_L \Psi_R^\dagger \Psi_R + \Psi_R^\dagger \Psi_R \Psi_L^\dagger \Psi_L \right) = 2g_0 \left( \hat{\Delta}_{+ij} \hat{\Delta}_{+ij}^\dagger + \hat{\Delta}_{-ij} \hat{\Delta}_{-ij}^\dagger \right).
\]

(42)

The part of the forward scattering which accounts for the interaction between the fermions of the same chirality cannot be expressed in terms of these four order parameters.

The effective coupling for CDW is always bigger than the effective coupling for the superconducting order parameter \( \hat{\Delta}_+ \):

\[
g_{\text{CDW}} > g_{\text{sc}}, \quad \text{where}
\]

\[
g_{\text{CDW}} = g + z_+ \tilde{g}_{2kF},
\]

(43)

\[
g_{\text{sc}} = \tilde{g}_{2kF} - g_0 = \zeta^{2K-2} \tilde{g}_{2kF} - g_0,
\]

(44)

\[
g_{\text{CDW}} = g + z_+ \tilde{g}_{2kF},
\]

(45)
and $z_\perp$ is the coordination number for a chain. Thus, at $T = 0$ for the perfect nesting the system is always in CDW phase with $\Delta_+$ order parameter phase being meta-stable ($g_{sc} > 0$) or unstable ($g_{sc} < 0$). Other order parameters, $\Delta_0$ and $\Delta_-\perp$, are unstable.

When the external pressure is applied the amplitude $t_2$ for hopping to the next-to-nearest chain begins to grow and spoils the Fermi surface nesting. This undermines stability of CDW and drives the transition temperature to zero \[8\]. Indeed, in the latter reference the following simple estimate for the density wave susceptibility was obtained:

$$\chi \propto \frac{1}{2\pi v_F} \times \begin{cases} \log \left( \frac{2v_F \tilde{\Lambda}}{T} \right), & \text{if } T > \tilde{t}_2 = \zeta^\theta t_2 \\ \log \left( \frac{2v_F \tilde{\Lambda}}{\tilde{t}_2} \right), & \text{if } T < \tilde{t}_2 = \zeta^\theta t_2. \end{cases} \quad (46)$$

The CDW transition temperature is derived by equating $(g + z_\perp \tilde{g}_{2k_F})\chi$ and unity. For $\tilde{t}_2 = 0$ it is:

$$T_{CDW} = v_F \tilde{\Lambda} \exp \left( -\frac{2\pi v_F}{g + z_\perp \tilde{g}_{2k_F}} \right). \quad (47)$$

If $\tilde{t}_2 > 0$ the transition temperature $T_{CDW}$ becomes smaller then $T_{CDW}^{(0)}$. It vanishes when $\tilde{t}_2 \propto T_{CDW}^{(0)}$. That is, exponentially small $\tilde{t}_2$ is enough to destroy CDW.

What happens after CDW is destroyed depends on the sign of $g_{sc}$. If $g_{sc} > 0$ the ground state is superconducting. Otherwise, it is the Fermi liquid. We can perform the same type of analysis we did above for CDW. The superconductivity is rather insensitive to the nesting properties of the Fermi surface. The susceptibility for $\Delta_+$ is equal to $(1/2\pi\alpha v_F)\log \left( (2v_F \tilde{\Lambda}) \right)$, where $\alpha$ is a constant of order of unity. The critical temperature is found to be:

$$T_c \propto v_F \tilde{\Lambda} \exp \left( -\frac{2\pi \alpha v_F}{g_{sc}} \right), \quad (48)$$

if $g_{sc} > 0$. Even when $g_{2k_F} < g_0$ the effective coupling $g_{sc}$ may be positive provided that the in-chain interaction is repulsive ($K < 1$) and the electron hopping anisotropy parameter $(\bar{u}\Lambda/t)$ is big:

$$\zeta^{2\zeta - 2} > \frac{g_0}{g_{2k_F}} \Leftrightarrow \left( \frac{\bar{u}\Lambda}{t} \right)^{(2-2\zeta)/(1-\theta)} > \frac{g_0}{g_{2k_F}} > 1. \quad (49)$$

For the system in the intermediate coupling regime this condition is likely to be satisfied.

It is interesting to note that the external pressure detrains not only CDW but the superconductivity as well. Under pressure the anisotropy parameter $(\bar{u}\Lambda/t)$ decays. The superconducting transition temperature gets smaller as the anisotropy decreases. At pressure
higher than some critical value the condition (49) is no longer satisfied. In this region the superconductivity is unstable and the ground state is the Fermi liquid.

The qualitative phase diagram is presented on the fig. 2. It shares two remarkable features with the phase diagram of the organic Q1D superconductors [1]: (i) the density wave phase and superconductivity have common boundary; (ii) the superconducting transition temperature vanishes at high pressure.

Our order parameter $\hat{\Delta}_+$ deviates from the more common version $\hat{\Delta}_0$. The order parameter $\hat{\Delta}_+$ was proposed quite some time ago [9]. Recently, this suggestion found further support in the renormalization group calculations of Ref. [3]. The advantage of $\hat{\Delta}_+$ stems from the fact that by having two electrons of a Cooper pair on different chains we avoid increasing in-chain potential energy.

The origin of the superconducting phase in our system is an interesting question worth discussing in more details. In conventional BCS model the superconductivity is stable because it minimizes the potential energy of the electron-electron interaction. We can make this claim rigorous by considering the following derivation. BCS hamiltonian density

$$H_{\text{BCS}} = T + V = \sum_\sigma \psi_\sigma^\dagger \left( \frac{\hat{p}^2}{2m} - \mu \right) \psi_\sigma - g \psi_\uparrow^\dagger \psi_\downarrow^\dagger \psi_\downarrow \psi_\uparrow$$

consists of two term: kinetic energy density $T$ and potential energy density $V$. At zero temperature the superconducting state energy density $E_{\text{sc}} = \langle H \rangle_{\text{sc}}$ is smaller then the normal energy density $E_n = \langle H \rangle_n$. This condensation energy density

$$E_c = E_n - E_{\text{sc}} \propto v T_c^2,$$

$$\nu = \pi^{-2} m^2 v_F,$$

$$v_F = \sqrt{2\mu/m},$$

is entirely due to depletion of interaction in the superconducting state:

$$\langle V \rangle_n - \langle V \rangle_{\text{sc}} > 0.$$

As for the kinetic energy it grows in the superconducting state:

$$\langle T \rangle_n - \langle T \rangle_{\text{sc}} < 0.$$

To prove this we will use Feynman formula which allows to calculate the ground state expectation value of any term $cO$ of the hamiltonian density:

$$c \langle O \rangle = c \frac{\partial E_{\text{gs}}}{\partial c},$$
where $\mathcal{E}_{gs}$ is the ground state energy. Therefore:

\[
\langle V \rangle_n - \langle V \rangle_{sc} = g \frac{\partial}{\partial g} \mathcal{E}_c, \tag{56}
\]

\[
\langle T \rangle_n - \langle T \rangle_{sc} = m^{-1} \frac{\partial}{\partial m^{-1}} \mathcal{E}_c, \tag{57}
\]

\[
\mathcal{E}_c \propto \omega_D^2 \mu^{1/2} m^{3/2} \exp(-\alpha \mu^{-1/2} m^{-3/2} g^{-1}), \tag{58}
\]

where $\omega_D$ is Debye frequency and $\alpha > 0$ is a constant of order unity. The inequalities (53) and (54) immediately follow from the expressions above. These inequalities mean that it is the electron-electron attraction which triggers BCS superconductivity. This fact is a very well known fact of the superconductivity mean-field theory.

However, in the system with strong repulsion, such as Q1D or high-$T_c$ materials, it is difficult to construct a mean-field superconducting phase which lowers the interaction energy. Our model for which we develop the consistent many-body approach can be used to discuss this issue beyond the mean-field approximation.

For our model it is easy to determine that the transverse forward scattering energy is increased and the exchange energy is decreased by the superconductivity. This result is a direct consequence of (42) and (41).

Contributions of other terms can be found with the help of Feynman formula. The condensation energy density is of the order of $-T_c^2/v_F$. Thus, differentiating the critical temperature (48) with respect to some coupling constant of (1) we can determine how a ground state energy contribution of a given term is modified by presence of the superconductivity. A derivative of the critical temperature with respect to a parameter $x$ is equal to:

\[
\frac{\partial}{\partial x} T_c \approx T_c v_F \frac{\partial}{\partial x} \log \left( \frac{g^2 k_F}{\pi} \frac{g_{sc}^2}{2K - 2} - g_0 \right), \tag{59}
\]

provided that $g_{sc} \ll v_F$. Combining this result with (45) we conclude that in the superconducting state the transverse hopping energy is higher:

\[
\left\langle -t \sum_{p(i,j)} \left( \psi_{p,i}^\dagger \psi_{p,j} + \text{h.c.} \right) \right\rangle_n - \left\langle -t \sum_{p(i,j)} \left( \psi_{p,i}^\dagger \psi_{p,j} + \text{h.c.} \right) \right\rangle_{sc} \propto g_{sc} T_c \frac{\partial}{\partial g \log \left( g_{2k_F} \frac{t}{\bar{u} \Lambda} \right)} < 0, \tag{60}
\]

and the in-chain potential energy is lower then in the normal state:

\[
\left\langle g \psi_{L,i}^\dagger \psi_{L,i} \psi_{R,i}^\dagger \psi_{R,i} \right\rangle_n - \left\langle g \psi_{L,i}^\dagger \psi_{L,i} \psi_{R,i}^\dagger \psi_{R,i} \right\rangle_{sc} \propto g \frac{T_c^2 g_{2k_F}^2}{g_{sc}^2} \log \left( \frac{t}{\bar{u} \Lambda} \right) \frac{\partial}{\partial g \left( \frac{2K - 2}{1 - \theta} \right)} > 0, \tag{61}
\]
since both $\log(t/\bar{u}\Lambda)$ and the derivative with respect to $g$ are negative.

We have proven that in our case the superconductivity is triggered by the electron-electron repulsion. This result is quite unexpected. It is has a many-body nature and cannot be obtained within a mean-field theory for the hamiltonian (1). This mechanism of superconductivity is very similar to the Kohn-Luttinger proposal. Classical Kohn-Luttinger mechanism predicts extremely low critical temperature. In our case, however, the effective coupling constant $g_{\text{sc}}$ is a non-analytical function of the bare parameters. As a consequence, our transition temperature (48) does not have to be small.

V. STRONG COUPLING REGIME

We have seen above that if $\theta > 1$ then $\Lambda$ is zero. This means that quasiparticles are not formed and it is more convenient to treat the system in terms of TL boson only. The bosonized hamiltonian (1) has the form:

$$H_{1d}^i = \frac{u}{2} \left( K (\nabla \Theta_i)^2 + K^{-1} (\nabla \Phi_i)^2 \right),$$

$$H_{ij}^{\perp} = \frac{g_{2kF}}{(2\pi)^2} \cos \sqrt{4\pi} (\Phi_i - \Phi_j).$$

In this formula both the transverse hopping term which is irrelevant in RG sense and the forward scattering term which is marginal are omitted. Their effect is small as compared with that of the strongly relevant exchange interaction, eq. (63).

The relevance of the exchange interaction indicates that at low temperature the system freezes into a state with the finite expectation value $\langle \Phi_i \rangle \neq 0$. This phase is CDW. It can be easily proved by bosonizing CDW order parameter: $\psi_{Li}^\dagger \psi_{Ri} \propto (2\pi a)^{-1} \exp(i\sqrt{4\pi} \Phi_i)$. The finite expectation value of the field $\Phi$ is inherited by CDW order parameter.

We describe this regime with the help of our variational wave function. Since $\Lambda = 0$ one can write the wave function in terms of TL bosonic field only:

$$|\text{Var}\rangle = \prod_{k>0,i} \frac{1}{\sqrt{2\pi \sigma_k^2}} \exp \left\{ - |\Phi_{ik}|^2 / 4\sigma_k^2 \right\}.$$ \hspace{1cm} (64)

This expression is a slight generalization of (11): in the latter equation the parameters $\sigma_k^2 = K/4|k|$. Here we do not fix $\sigma_k^2$. Instead, they will be determined variationally. Variational energy is:

$$E^V/(LN_{\perp}) = u \int_0^\Lambda \frac{dk}{2\pi} \left( \frac{K}{8\sigma_k^2} + 2k^2 \sigma_k^2 \right) - g_{2kF} \Lambda^2 \exp \left\{ -8 \int_0^\Lambda dks_k^2 \right\}.$$ \hspace{1cm} (65)
Minimizing this energy with respect to $\sigma_k^2$ we find:

$$\sigma_k^2 = \frac{Ku}{4\sqrt{u^2k^2 + \Delta_{CDW}^2}}, \quad (66)$$

$$\Delta_{CDW}^2 = 8\pi g_{2k_F} K u \Lambda^2 \exp \left\{ -2K \int_0^{u\Lambda} \frac{d\varepsilon}{\sqrt{\varepsilon^2 + \Delta_{CDW}^2}} \right\} \propto g_{2k_F} u \Lambda^2 \left( \frac{\Delta_{CDW}}{u\Lambda} \right)^{2K}. \quad (67)$$

The quantity $\Delta_{CDW}$ has the meaning of the excitation gap due to CDW order. This gap, together with the transition temperature, can be found by solving the last equation:

$$T_{CDW} \propto \Delta_{CDW} \propto u\Lambda \left( \frac{g_{2k_F}}{u} \right)^{1/(2-2\kappa)}. \quad (68)$$

The variational energy is:

$$E^V / (LN_L) \propto \Delta_{CDW}^2 / u. \quad (69)$$

These results are correct when $H^\perp$ couples only those chains which are nearest neighbors. The next-to-nearest neighbor coupling frustrates CDW phase. We will not discuss the effect of the frustration in this paper.

Finally, let us discuss cross-over from strong to intermediate coupling regime. Such cross-over occurs when the intermediate coupling Fermi liquid energy, eq. (16), becomes equal to the strong coupling CDW energy, eq.(69):

$$\tilde{t}^2 / v_F \propto \Delta_{CDW}^2 / u \quad \text{or} \quad \left( \frac{t}{u\Lambda} \right)^{1/(1-\theta)} \propto \left( \frac{g_{2k_F}}{u} \right)^{1/(2-2\kappa)}. \quad (70)$$

This equation defines $\theta_c(t, g_{2k_F}) < 1$ at which the cross-over takes place. At small $\theta < \theta_c$ the system behaves as the Fermi liquid whose properties we discussed in the previous sections. When $\theta > \theta_c$ the expression (17) is no longer applicable: the necessary requirement for smallness of the energy associated with symmetry breaking is violated. The expression (69) has to be used instead.

Fig.3 shows how the strong coupling regime at big $\theta$ is replaced by the intermediate coupling regime at smaller $\theta$. The transition temperature of CDW, eq.(68), drops sharply and becomes exponentially small, eq.(47), as $\theta$ gets smaller then $\theta_c$. This diagram was discussed in [10] for a similar model.

VI. CONCLUSIONS

We propose in this paper the variational wave function for Q1D system. Our procedure key ingredient is the splitting of TL bosons into high-momentum and low-momentum modes.
While high-momentum modes are in their ground state the low-momentum modes form quasiparticles which delocalize in the transverse directions.

Our method can be viewed as a variational implementation of the lowest order RG scaling near TL liquid fixed point. When the transverse hopping amplitude becomes of the order of $u \Lambda$ the scaling must be stopped. The renormalized hamiltonian should be treated as the hamiltonian for the quasiparticles.

Our method gives us a possibility of computing different Green’s functions beyond RG using standard diagrammatic technique. As an example we calculated the lowest order self-energy for the one-particle propagator.

Depending on the strength of the in-chain interaction and the anisotropy the system may be in one of three regimes: strong, intermediate or weak coupling. In the strong coupling regime quasiparticles are not formed and the system is better described in terms of TL bosons. In weak and intermediate coupling regime the low-lying degrees of freedom are quasiparticles. The ground state of these fermions may be either Fermi liquid, the superconductivity or CDW. The phase diagram of our Q1D model looks very similar to that of the organic Q1D superconductors.

Unlike classical BCS superconducting phase, the one in our model is stabilized without any attraction between the electrons. It is similar to Kohn-Luttinger superconductivity. However, our effective coupling constant is bigger then that of Kohn-Luttinger. This guarantees that the critical temperature in our model is not unacceptably small.

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FIG. 1: Lowest order contribution to the self-energy of the quasiparticle.

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FIG. 3: The energy scale associated with transverse hopping $\tilde{\Lambda}$ decreases when $\theta$ grows. The CDW transition temperature $T_{\text{CDW}}$ increases as $\theta$ grows. At $\theta_c$ where both energy scales are of the same order the cross-over from the intermediate to strong coupling occurs.