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# RENORMALIZATION GROUP APPROACH TO THE ONE-DIMENSIONAL 1/4-FILLED HUBBARD MODEL WITH ALTERNATING ON-SITE INTERACTIONS

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# 1 Introduction

The remarkable discovery of high-Tc superconductivity [1] in Cu-O compounds has raised the interest in the physics of correlated electrons in low dimensions. For better understanding of the high-Tc superconductivity mechanism it is interesting to investigate one-dimensional analogues of Cu-O planes.

Emery proposed a one dimensional version [2] of two-band copper-oxide model [3]. In Emery's model two essential features distinguishing the Cu and O sites in real systems are incorporated: 1. the chemical aspect - the hole has different on-site energies on copper and oxygen sites and 2. the dynamical aspect - there are different on-site interactions between two holes on copper sites ($U_a$) and on oxygen ($U_b$). To investigate the influence of the dynamical nonequivalence of copper and oxygen sites Japaridze et al. [4] considered a rather formal 1D version of the Cu-O chain, namely the one-band Hubbard model with different on-site interaction on even and odd sites. This model was investigated in the framework of standard weak coupling approach using a boson representation theory.

The another method by which insight can be gained into the problem of interacting fermions is to use the renormalization group (RG) [5], [6], [7]. It isn't without interest to consider the same model as in [4] by RG technique.

As will be shown in **2**, the continuum Hamiltonian of the model has a general form, describing the one-dimensional system of interacting fermions. The Hamiltonian of the same form has been considered by Kimura [5] using the conventional field-theoretical renormalization group. Solyom [6] performed the second order scaling procedure, using the bandwidth cutoff, to more general case, when the forward scattering process between particles from the same branch was presented. According to Solyom, taking into account this process substantially changes results. Unlike [6], Rezayi et al. [7] have shown, that if one modifies the term corresponding backward scattering and Umklapp process, replacing them by effective spin and charge carrying interactions, one gets the theory with momentum transfer cutoff. In this case, the effect of the forward scattering process between particles from the same branch is absorbed to a Fermi velocity renormalization and couplings, which couple the spin-density degrees of freedom scale independently of the couplings, which couple the charge-density degrees of freedom.

In our calculation, we shall neglect the forward scattering process between particles from the same branch and assuming that the forces are short range, use the bandwidth cutoff. In this case, the Lie equations for the coupling constants decouple into two sets and are analogous to those obtained by using the momentum transfer cutoff [7]. As will be shown in **4.** the scattering processes responsible to a Fermi velocity ranormalization can only lead to the difference between the degrees of the divergency of CDW and SDW response functions.

## 2 The model

The Hamiltonian describing the model has the following form:

$$H = -t\sum_{n,\alpha} c^{+}_{n,\alpha}(c_{n+1,\alpha} + c_{n-1,\alpha}) + \frac{1}{2}\sum_{n,\alpha}[U + (-1)^n V]\rho_{n,\alpha}\rho_{n,-\alpha} + \quad (1)$$

$$+ \sum_{n,\alpha,\beta}[V_1\rho_{n,\alpha}\rho_{n+1,\beta} + V_2\rho_{n,\alpha}\rho_{n+2,\beta}]$$

where $c^{+}_{n,\alpha}(c_{n,\alpha})$ is a creation (annihilation) operator for a particle of spin $\alpha$ in the Wannier state localized at the $n$th lattice site, $\rho_{n,\alpha} = c^{+}_{n,\alpha}c_{n,\alpha}$ and

$$U = \frac{1}{2}(U_a + U_b)$$

$$V = \frac{1}{2}(U_a - U_b)$$



where $U_a(U_b)$ describes on-site interaction on even (odd) lattice sites and $V_1$ and $V_2$ describe the interactions between particles on nearest and next-nearest neighbor sites, respectively.

The continuum limit of the Hamiltonian (1) can be taken by approximating the spectrum $-2t\cos k$ by linear spectra around $\pm k_F$ and using the correspondence:

$$c_{n,\alpha} \rightarrow exp(ik_F n)\psi_{1,\alpha}(x) + exp(-ik_F n)\psi_{2,\alpha}(x) \quad (2)$$

where the fermion field $\psi_{1(2),\alpha}(x)$ describes the particles around Fermi point $+(-)k_F$.

In the case of quarter-filled band, the dynamical nonequivalence of sites becomes important and leads to the appearance of Umklapp processes [4]. The continuum limit Hamiltonian has the form:

$$H = -iv_F\sum_{\alpha}\int dx[\psi^{+}_{1,\alpha}\partial_x\psi_{1,\alpha} - \psi^{+}_{2,\alpha}\partial_x\psi_{2,\alpha}] + \quad (3)$$

$$+\pi v_F\sum_{\alpha,\beta}\int dx\Big\{[g_{1\|}\delta_{\alpha,\beta} + g_{1\perp}\delta_{\alpha,-\beta}]\psi^{+}_{1,\alpha}\psi^{+}_{2,\beta}\psi_{1,\beta}\psi_{2,\alpha} +$$

$$+[g_{2\|}\delta_{\alpha,\beta} + g_{2\perp}\delta_{\alpha,-\beta}]\psi^{+}_{1,\alpha}\psi^{+}_{2,\beta}\psi_{2,\beta}\psi_{1,\alpha} + \frac{g_3}{2}\delta_{\alpha,-\beta}(\psi^{+}_{1,\alpha}\psi^{+}_{1,\beta}\psi_{2,\beta}\psi_{2,\alpha} + \text{h.c.})\Big\}$$

The Hamiltonian (3) has a general form describing the interacting fermion system in 1D. The terms with coupling constants $g_{1\|}$, $g_{1\perp}$ and $g_{2\|}$, $g_{2\perp}$ correspond to the backward and forward scattering processes,respectively and the terms with $g_3$ - to the Umklapp process. In the (3) the processes with coupling constants $g_{1\|}$ and $g_{2\|}$ are indistinguishable and we can choose $g_{2\|} = g_{2\perp}$, without loss of generality. This leads to the following values of the spin independent bear coupling constants:

$$g_1 \equiv g_{1\|} = g_{1\perp} = \frac{U - 2V_2}{\pi v_F};\; g_2 \equiv g_{2\|} = g_{2\perp} = \frac{U + 2V_1 + 2V_2}{\pi v_F};\; g_3 = \frac{V}{\pi v_F} \quad (4)$$

In obtaining (3), the terms corresponding to forward scattering processes, in which both incoming particles are from the same branch, were omitted.

## 3 Renormalization group technique

The multiplicative renormalization group has been used in the field theory for a long time to eliminate divergences [8]. This method has two main aspects. The first one is that starting from a perturbational calculation a partial summation is obtained by solving the group equations and second one - a set of equivalent problems can be found which are described by Hamiltonian of similar form. If there is a model among the equivalent ones which can be solved, the solution of the original problem can also be obtained.

The renormalization group treatment of the problem of interacting fermions in 1D was given by Menyhard and Solyom [9]. Here we will briefly present the ideas applied to the 1D Fermi gas.

For an unambiguous definition of the model it is necessary to specify the cutoff procedure which determines the domains of admissible values of the electron momenta. If the interactions are short range we have effectively only one limit on momenta and got a theory with bandwidth cutoff. In the general case, when the long-range forces are also presented, theory needs two cutoffs, one as bandwidth and one on momentum transfer [10]. Assuming that the forces are short range in our case, we shall use the bandwidth cutoff.

At first let us write the auxiliary Green's function $d$ and four-pointed vertex function $\tilde{\Gamma}_i$ in the following way:

$$G(k_F,\omega) = d(\frac{\omega}{E_0}, g_i) G_o(k_F,\omega) \tag{5}$$

$$\Gamma_{\alpha\beta\gamma\delta}(\omega) = g_1\tilde{\Gamma}_1(\omega)\delta_{\alpha\gamma}\delta_{\beta\delta} - g_2\tilde{\Gamma}_2(\omega)\delta_{\alpha\delta}\delta_{\beta\gamma} \tag{6}$$

for process with momentum conversation and



$$\Gamma_3 = g_3\tilde{\Gamma}_3(\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{\alpha\delta}\delta_{\beta\gamma}) \tag{7}$$

for Umklapp process, where $E_0$ is a bandwidth cutoff. For the following discussion the parameter $g_4 = g_1 - 2g_2$ is also useful.

If the cutoff $E_0$ is changed to $E_0'$ and simultaneously the coupling constants $g_i$ are transformed to certain new values

$$g_i' = z_i' g_i$$

then the functions $d$ and $\tilde{\Gamma}_i$ are multiplicatively transformed to

$$d(\frac{\omega}{E_0'}, g_i') = z d(\frac{\omega}{E_0'}, g_i) \tag{8}$$

$$\tilde{\Gamma}_i(\frac{\omega}{E_0'}, g_i') = z_i^{-1}\tilde{\Gamma}_i(\frac{\omega}{E_0}, g_i) \tag{9}$$

Moreover, requiring the invariance of quantity $g_i\tilde{\Gamma}_i d^2$, which is an appropriately renormalized vertex [11], only four of renormalization constants $z_i$, $z_i'$ and $z$ are independent and we have $z_i' = z_i/z^2$

The scaling equations for $d, \tilde{\Gamma}_i$ and $g_i'$ can be written in a common form as:

$$C(\frac{\omega}{E_0'}, g_i') = zC(\frac{\omega}{E_0}, g_i) \tag{10}$$

For any quantity obeying the condition (10) a Lie differential equation of the form:

$$x\frac{\partial}{\partial x}\ln C(x, g_i) = \frac{\partial}{\partial \xi}\ln C(\xi, g_i')\Big|_{\xi=1} \tag{11}$$

can be derived, where $x = \omega/E_0$.

The right-hand side of Lie equation can be calculated by perturbation theory. If the invariant couplings $g_i(x) \equiv g_i'$ are small for an arbitrary change of the scaling energy the quantity determined from the solution of the Lie equation using a few terms of the perturbation series will present a good approximation in the whole energy range. If, however, the invariant couplings become of the order of unity while scaling energy goes towards lower energies, the right-side of the Lie equation breaks down and only qualitative results can be obtained.

### 3.1 First-order renormalization

Calculating the right-hand side of the Lie equations in the second-order of the perturbation theory the following equations for invariant couplings can be obtained

$$x\frac{\partial}{\partial x}g_1(x) = g_1^2(x) \tag{12}$$

$$x\frac{\partial}{\partial x}g_4(x) = g_3^2(x) \tag{13}$$

$$x\frac{\partial}{\partial x}g_3(x) = g_4(x)g_3(x)$$

The first order scaling is equivalent to summing up the leading terms and these equations are exactly analogous to those obtained in [12] by parquet approximation. Let us first analyze the model (1) in the case $V_1 = V_2 = 0$ In this case the solutions of Eq.(12) and (13) with boundary conditions $g_1(0) = U/\pi v_F$, $g_4(0) = -U/\pi v_F$ and $g_3(0) = V/\pi v_F$ have the form:

$$g_1(x) = \frac{U}{1-Ut} \tag{14}$$

where $t = \ln x$;

$$g_4(x) = \frac{-U}{1+Ut},\ g_3(x) = \frac{V}{1+Ut} \tag{15}$$

for $U^2 = V^2$;

$$g_4(x) = -D\coth D(t_0 - t),\ g_3(x) = \frac{D\text{sgn}V}{|\sinh D(t_0 - t)|} \tag{16}$$



for $U^2 > V^2$, where $t_0 = 1/D\text{arccoth}(U/D)$;

$$g_4(x) = -D\cot D(t_0 - t),\ g_3(x) = \frac{D\text{sgn}V}{|\sin D(t_0 - t)|} \tag{17}$$

for $U^2 < V^2$, where $t_0 = 1/D\text{arccot}(U/D)$ .

These equations show that, at certain values of bare couplings, the poles appear in the expressions of the invariant coupling constants. This singular behavior of invariant couplings doesn't indicate the phase transition at finite temperature, which is impossible in one dimensional system [13]. The existence of the poles in expressions (14)–(17) indicates that at low temperatures the interactions become strong and this approximation is no longer valid. In [12] Dzyaloshinsky and Larkin, comparing their result to exact solution obtained by Gauden [14], emphasized, that the poles in the expressions of the invariant couplings can indicate the appearance of the gap in the one particle excitation spectrum. It is known, that $g_1$ and $(g_3, g_4)$ describe the spin and charge part of the system respectively [15], [7], thus we can expect that the spin (charge) gap exists when there is a pole in the expression for $g_1$ (($g_3$, $g_4$)). Thus the charge gap exists in all sectors except **A**, while the spin gap exists in the sectors **A**, **B**, **E** (see **Fig.1**).

### 3.2 Second-order renormalization

The second-order renormalization corresponds to considering next to leading logarithmic corrections and thereby to taking into account fluctuation effects. In the limit of third order of perturbation theory for $d$ and $\tilde{\Gamma}_i$, the following Lie equations for invariant couplings can be obtained:

$$x\frac{\partial}{\partial x}g_1(x) = g_1^2(x)[1 + \frac{1}{2}g_1(x)] \tag{18}$$

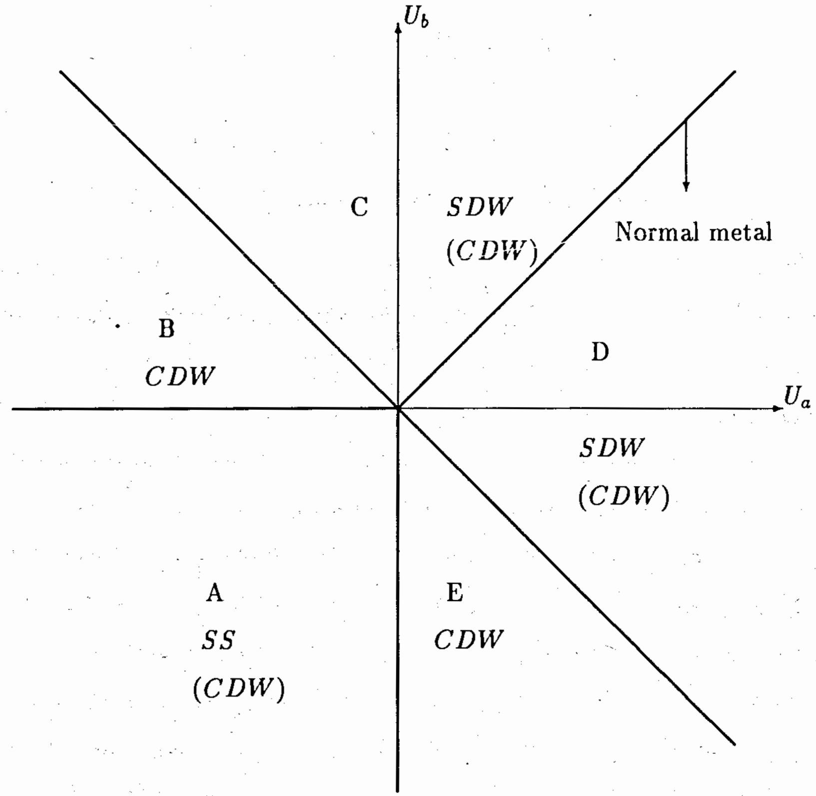


**Fig.1** The ground-state phase diagram of the model (1) ($V_1 = V_2 = 0$). The response functions corresponding to the phases shown in the parentheses have a lower degree of divergence than the others.

$$x\frac{\partial}{\partial x}g_4(x) = g_3^2(x)[1+\frac{1}{2}g_4(x)] \tag{19}$$

$$x\frac{\partial}{\partial x}g_3(x) = g_4(x)g_3(x)[1+\frac{1}{4}g_4(x)] + \frac{1}{4}g_4^3(x)$$

The solutions of these equations can be obtained only in an implicit form. They are the smooth functions of energy and tend to the saturation values, fixed points, at $\omega = 0$. The values of the fixed points can be obtained from



zeros of the right-hand sides of the Lie equations by using the following arguments:

*a*). From eq.(19): $x\frac{\partial}{\partial x}g_1(x) \leq 0$ for $g_1(x) \geq -2$; *b*). From eq.(20):

$x\frac{\partial}{\partial x}g_4(x) \leq 0$ for $g_4(x) \geq -2$ and $\frac{g_4^2 - g_3^2}{g_4 + 2} = c$, where $c$ is a constant.

The values of the fixed points depend on the relation between bare coupling constants and they are presented in **Table 1.**

**Table 1.** The values of the fixed points for invariant coupling constants. The letters A...C describe the same region as in Fig.1 and $\gamma = (c+\sqrt{c^2+8c})/2$

| | A | B | C | D | E |
|---|---|---|---|---|---|
| $g_1(0)$ | -2 | -2 | 0 | 0 | -2 |
| $g_2(0)$ | $-1-\gamma/2$ | 0 | 1 | 1 | 0 |
| $g_3(0)$ | 0 | 2 | 2 | -2 | -2 |
| $g_4(0)$ | $\gamma$ | -2 | -2 | -2 | -2 |

### 3.3 Response functions and ground-state phase diagram

The symmetry of the ground-state can be found by investigation of various response functions which are expected to be singular. These quantities are the charge-density (CDW) and spin-density (SDW) waves with wave-vector $k = 2k_F$, the singlet-superconductor (SS) and triplet-superconductor (TS) response functions with wave-vector $k = 0$ [16].

In the case of 1/4-filled band the periodicity of the CDW and SDW is equal four lattice constant and it is possible to introduce two separate sets of order parameters describing the fluctuations of the charge and spin density on even

($a$) and odd ($b$) sublatticies. In the real space and time representation general formula for these functions is

$$\Phi(x,t) = -i\theta(t) < [U(x,t)U^+(0,t)] > \qquad (20)$$

where $U(x,t) = \sum_\alpha[\psi^+_{1,\alpha}(x,t)\psi_{2,\alpha}(x,t) + \psi^+_{2,\alpha}(x,t)\psi_{1,\alpha}(x,t)]$ for the charge-density response function $N(x,t)$; $\psi^+_{1,\uparrow}(x,t)\psi_{2,\downarrow}(x,t) + \psi^+_{2,\uparrow}(x,t)\psi_{1,\downarrow}(x,t)$ for the spin-density response function $\chi(x,t)$ and $\psi^+_{1,\uparrow}(x,t)\psi_{2,\downarrow(\uparrow)}(x,t)$ for singlet (triplet)-superconductor response function $\Delta_{s(t)}(x,t)$

The Fourier-transformed response functions don't satisfy the criterion of multiplicative renormalization, Solyom [16] introduced the auxiliary renormalizable functions defined by

$$\overline{\Phi}_i(\omega) = \frac{\partial\Phi_i(\omega)}{\partial\ln(\omega)}$$

where $\Phi_i(\omega)$ is one of the above considered response functions. In the limit of second order of perturbation theory the following Lie equations for these renormalizable response functions can be obtained:

$$\frac{\partial\overline{N}_{a(b)}(x)}{\partial\ln(x)} = 2g_1(x) - g_2(x) + (-)g_3(x) + F(x) \qquad (21)$$

$$\frac{\partial\overline{\chi}_{a(b)}(x)}{\partial\ln(x)} = -g_2(x) - (+)g_3(x) + F(x) \qquad (22)$$

$$\frac{\partial\overline{\Delta}_s(x)}{\partial\ln(x)} = g_1(x) + g_2(x) + F(x) \qquad (23)$$

$$\frac{\partial\overline{\Delta}_t(x)}{\partial\ln(x)} = g_2(x) - g_1(x) + F(x) \qquad (24)$$

where

$$F(x) = \frac{1}{2}(g_1^2(x) + g_2^2(x) - g_1(x)g_2(x) + \frac{1}{2}g_3^2(x))$$

and $\overline{N}_a(x)$ and $\overline{N}_b(x)$ ($\overline{\chi}_a(x)$ and $\overline{\chi}_b(x)$) describe the CDW (SDW) located on $a$ and $b$ sublatticies , respectively and they are different only in a sign of $g_3$, the changing $a \rightarrow b$ is equivalent to change the sign of Umklapp processes.



In the limit $\omega \rightarrow 0$ the asymptotic expressions of response functions are obtained as

$$\Phi_i(\omega) \propto \overline{\Phi}_i(\omega) \propto (\frac{\omega}{E_0})^{\alpha_i}$$

The critical exponents $\alpha_i$ can be obtained by putting the fixed points of invariant couplings in the right-hand side of Eq.(21-24) and they are presented in **Table 2**

**Table 2** The critical exponents $\alpha_i$

| | A | B | C | D | E |
|---|---|---|---|---|---|
| $N_{a(b)}$ | -3/2+γ/2 | 1 (-3) | 5 (-3/2) | -3/2 (5/2) | -3 (1) |
| $\chi_{a(b)}$ | 5/2+γ/2 | 1 (5) | -3/2 (5/2) | 5/2 (-3/2) | 5 (1) |
| $\Delta_s$ | -3/2-γ/2 | 1 | 5/2 | 5/2 | 1 |
| $\Delta_t$ | 5/2-γ/2 | 1 | 5/2 | 5/2 | 1 |

According to singularities in the response functions let us summarize the ground-state phase diagram. In the sector **A** the CDW and SS response functions are divergent. The dominant singularity is in the singlet-superconductor response.

In the sectors **B** and **E** only CDW response, located on the sublattice with lower on-site interaction, is divergent.

There is coexistence of CDW and SDW in the sectors **C** and **D**. The CDW is still located on the sublattice with lower on-site interaction while the SDW is located on the other one.

In the case of nonalternating chain, $g_3 = 0$, $g_4$ doesn't renormalize and system has the properties of normal metal for $U > 0$ and singlet-superconductor for $U < 0$.

The ground-state phase diagram obtained here is exactly analogous to that obtained by boson representation theory in [4].

# 4 Scaling to the exactly soluble models

The renormalization group and scaling arguments presented in **3** establish a relationship between the original problem and a set of problems in which the coupling constants have the somewhat different values. If an exactly soluble model appears among these equivalent systems, the physical behaviors of the original model can be predicted by using the scaling arguments.

From Tab.1 one can easily see that depending on relation between the bare couplings the model can be scaled to Tomonaga [17] or Lutter-Emery (LE) [18] model and the ground-state phase diagram can be obtained by using their results [10].

**(i).** In the sector **A** (see**Fig.1**), $g_1(1) < 0$, $g_1(1) - 2g_2(1) \geq |g_3(1)|$, the spin part of the Hamiltonian scales to the LE line and there is a gap in the spin part of the excitation spectrum. The charge part scales to a Tomonaga model and the Umklapp processes have no influence. Only the CDW and SS responses can be divergent. The dominant singularity is in the latter.

**(ii).** For $g_1(1) > 0$, $g_1(1) - 2g_2(1) < |g_3(1)|$, sectors **C**, **D**, the situation is reversed concerning the spin and charge parts of the Hamiltonian. The gap is in the charge part and CDW and SDW responses show a singular behavior. The latter is more singular. The difference between singularity in CDW and SDW responses is caused by Fermi velocity renormalization [10] for which scattering processes omitted in (2) is responsible [7].

**(iii).** In the sectors **B** and **E**, $g_1(1) < 0$, $g_1(1) - 2g_2(1) < |g_3(1)|$, the Hamiltonian scales to the LE line, there is a gap in both charge and spin parts and only charge-density response function is divergent.



## 4.1 The role of intersite interactions

Taking into account the effects of intersite interactions leads to the renormalization of bare coupling constants Eq.(4). Let us consider the phase diagram for the arbitrary sign of the bare coupling constants, not restricting ourselves by realistic case, when $U_a$, $U_b$, $V_1$ and ;$V_2 > 0$.

In the case of extended model the spin and charge gaps exist in the case when $U - 2V_2 < 0$ and $-(U + 4V_1 + 6V_2) \geq |V|$, respectively.

**(i).** Now the situation discussed in **4.(i)** takes a place when

$$U - 2V_2 < 0 \text{ and } -(U + 4V_1 + 6V_2) \geq |V|$$

and the ground-state of the system is the same as in sector **A**.

**(ii).** When the bare couplings constants satisfy the condition:

$$U - 2V_2 \geq 0 \text{ and } -(U + 4V_1 + 6V_2) < |V|.$$

in the extended model,the same response functions as in sectors **B** and **E** are divergent.

**(iii).** The system has the same ground-state as in sectors **C** and **D** when

$$U - 2V_2 < 0 \text{ and } -(U + 4V_1 + 6V_2) < |V|.$$

**(iiii).** Unlike to the case $V_1 = V_2 = 0$, when intersite interactions are presented, the Hamiltonian scales to the Tomonaga model when:

$$U - 2V_2 \geq 0 \text{ and } -(U + 4V_1 + 6V_2) \geq |V|$$

There is no gap in either the charge or spin parts of the Hamiltonian and the singlet- and triplet-superconductor responses are divergent.

## 5 Summary

The one-dimensional 1/4-filled Hubbard model with alternating on-site interactions has been considered in the weak coupling approach using the Ranormalization group technique. The ground-state phase diagram obtained in the limit of second order renormalization is exactly analogous to that obtained by a boson representation method. Depending on the sign and relative values of the bare coupling constants, there is a gap in the spin or charge excitation spectrum and the model system tends to superconducting or antiferromagnetic order at $T = 0$, with doubled period. It is shown by scaling to exactly soluble models that the terms corresponding to scattering processes, in which both incoming particles are from the same branch lead to the difference between the degrees of the divergency of CDW and SDW response functions. The role of interaction between particles on nearest and next-nearest neighbor sites is also considered.



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