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Abstract The theory of a 1-D metal with a half-filled band is developed on the base of the simplest model with constant couplings of a finite range. Renormalization group method is applied. Within the framework of the next divergent logarithmic accuracy the finite charge renormalization is performed. The behavior of the system near the Fermi surface at low temperature are predicted to be of universal charactor. In particular, the Green's function and the vertex functions should obey the power law. The power indices are evaluated in the various case of the bare coupling constants. The theory yields results in accord with the exact theorem about the phase transitions in 1-D systems.

§ 1. Introduction

One-dimensional metallic systems have been much interested experimentally and theoretically. However, there have been known only a few confirmative results[1]. Because of the serious difficulties in studying the 1-D attractive electrons in metals due to the existence of the mutually coupled superconducting and Peierls instabilities the interpretations of the giant conductivity recently observed in TCNQ series have been very controversy[2].

Some years ago, BYCHKOV, GOR'KOV and DZYALOSHINSKII[3] studied by a parquet diagram method the coupled two channel problem in 1-D Fermi systems with a simple model and concluded the occurrence of the simultaneous phase transition of the superconducting and Peierls types at some finite temperature. However, this conclusion is by no means acceptable in view of the theorem[4,5] which dose not permit any type of off-diagonal long range order to exist in 1-D system at finite temperture.

In the author's recent note[6] the renormalizability of B.G.D's 1-D model[3] was pointed out, and the multiple renormalization group (MRG) method[7] was used to study this model. The result there, being valid within the most divergent logarithmic terms, indicated the occurrence of the finite temperature instabilities completely analogous to

those of the parquet analysis[3].

More recently, MENYHART and SOLYOM[8] reported their calculations by the same method but taking into account the contributions up to the next divergent terms. The effect of the density and spin fluctuations considered in the next order terms critically suppressed the above mentioned intabilities, thus the absence of the phase transitions except at the ground state was concluded.

The purpose of the present paper is to extent the investigation to the asymptotic low temperature properties of the 1-D metals with half-filled bands. As was pointed out by DZYALOSHINSKII and LARKIN[9], the umklapp processes in such systems strongly affect the stability of the ground states; normal, antiferromagnetic or superconducting. Clearly, the most divergent approach which led to the finite temperature instability[9] is not sufficient. Therefore the problem for the present case remains still open.

In §2 the model to include the umklapp process is explained and the MRG method is briefly outlined. In §3 the perturbation series for the electron self-energy and the vertex function up to the third order terms are studied within the logarithmic accuracy. In §4 the solutions for the MRG equations are studied. As a result, the invariant charges which are the effective expansion parameters of the theory show some finite behaviors over the whole range of their argument and the asymptotic forms of the Green's function (GF) and the vertex function (VF) are of a power type. In §5 the results are interpreted and discussed.

§2. The model and formulations of MRG method

Let us consider the 1-D metallic electron system in a periodic lattice, which is described by the interaction;

$$H=-\sum V(p_1,...,p_4)\, a^+_{p_1\alpha} a^+_{p_2\beta} a_{p_4\beta} a_{p_3\alpha} \Delta_{p_1+p_2,\, p_3+p_4}. \tag{1}$$

where

$$\Delta_{p_1+p_2,\, p_3+p_4} = \begin{cases} 1 & \text{for } p_1+p_2=p_3+p_4+G, \\ 0 & \text{otherwise,} \end{cases} \tag{2}$$

G is a reciprocal lattice vector. If the band is half-filled

$$G=4np_F\ ,\ n=0,\ \pm1,\ \pm2,.....,$$

where p_F is the Fermi momentum of the electron. With this in mind we consider the simple case of $V(p_1,...,p_4)$ as;

$$V(+--+)=g_1,$$

$$V(+-+-)=g_2, \tag{3}$$
$$V(++--)=g_3,$$

where the sign + or − means that the corresponding momentum p_i lies within the range of width D/v (v is the Fermi velocity of the electron) around the plus or minus side of the Fermi surface. The coupling constant g_3 corresponds to the umklapp process.

The renormalizability of our model can be readily verified by considering the diagram index K for any connected graph in the perturbation series. In our case it is given by

$$K=2-N/2$$

with N the number of the external lines. One can see that the situation concerning this index K is completely analogous to the case of the kondo effect, and the proof for the renormalizability is the same as that given by ABRIKOSOV and MIGDAL[10] in the latter case.

For the model above described the most important cases for VF are written as;

$$\Gamma\alpha_1\alpha_2\alpha_3\alpha_4(+---)=g_1\Gamma_1\delta\alpha_1\alpha_3\delta\alpha_2\alpha_4-g_2\Gamma_2\delta\alpha_1\alpha_4\delta\alpha_2\alpha_3, \tag{4}$$
$$\Gamma\alpha_1\alpha_2\alpha_3\alpha_4(++--)=g_3\Gamma_3(\delta\alpha_1\alpha_3\delta\alpha_2\alpha_4-\delta\alpha_1\alpha_4\delta\alpha_2\alpha_3)$$

(see Fig.1), and the full GF;

$$G(p)=d(p)/(\epsilon-\xi_p), \tag{5}$$

where $\xi_p=v\mid p-p_F\mid$ and

$$d(p)=(1-G_0\Sigma)_p^{-1}. \tag{6}$$

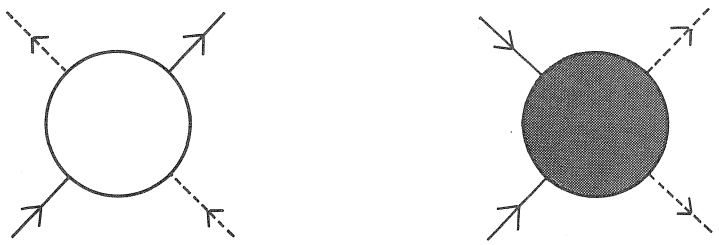


Fig.1. The full vertex part corresponding to (4) in the text. The full line represents the electron with momentum$\sim p_F$ and the broken line with momentum$\sim -p_F$.

The scale-invariant charges in our theory are given by

$$\Psi_i(x,\ u,\ g)=g_i d^2(x,\ u,\ g)\Gamma_i(x,\ u,\ g)/\pi v, \tag{7}$$

where x and u are the characteristic energy of the electron and the cutoff D which are suitably scaled, and $g=(g_1,\ g_2,\ g_3)$, the set of the bare couplings. These invariant charges must satisfy the set of Lie equations;

$$z\frac{\partial}{\partial z}\Psi_i(z,g)=\Phi_i(z,g), \tag{8}$$

where

$$\Phi_i(z,g)=\frac{\partial}{\partial\xi}\Psi_i(\xi,\frac{1}{z},g)\mid_{\xi=1}, \tag{9}$$

$$z=x/u.$$

We have assumed the following subsidiary condition must be fulfilled by d and Γ_i;

$$F(1,u,g)=1, \qquad F=d \text{ or } \Gamma_i, \tag{10}$$

Hence,

$$\Psi_i(1,u,g)=g_i/\pi v. \tag{11}$$

Generally, we can consider the following two conceptually different possibilities; the case I, the finite charge renormalization,

$$\int_{g_i}^{\lambda_i}\frac{dg_i}{\Phi_i(g)}=\infty, \tag{12}$$

where

$$\lambda_i=\Psi_i(0,g);\qquad \text{finite},$$

and the case II, the infinite charge renormalization,

$$\int_{g_i}^{\infty}\frac{dg_i}{\Phi_i(g)}=M, \qquad (M \text{ is finite or infinite}). \tag{13}$$

In the case I of the finite charge renormalization the function Φ_i has a sufficiently strong zero at $g_i=\lambda_i$. In the following we shall see that the final results will bring us to the case I whereas the case II will be met in the intermediate step of the insufficient lower approximation.

It should be noticed that the Lie equations analogous to Eq(8) must hold for any other renormalization-multiplicative quantities with some modifications, in particular, for d and Γ_i;

$$z\frac{\partial}{\partial z}\ln d(z,g)=\frac{\partial}{\partial\xi}d\ (\xi z,\Psi(z,g))\mid_{\xi=1}, \tag{14}$$

$$z_i\frac{\partial}{\partial z_i}\ln\Gamma_i(\cdots\cdots,z_i,\cdots\cdots,g)=\frac{\partial}{\partial\xi}\Gamma_i(\cdots\cdots,\xi z_i,\cdots\cdots,\Psi(z,g))\mid_{\xi=1}. \tag{15}$$

Once Ψ are known these equations are solved by quadrature.

§3, Perturbational determination of the scaling functions

In the MRG method the dynamical aspects of the system under consideration are embodied in the scaling functions. The method employed here to determine the functions ϕ and also the functions in the right hand sides of Eqs (14) and (15) is the conventional diagrammatic expansion of VF and the self energy of the electron which is considered to be reliable at least in the neighborhood of the cutoff D and in the weak coupling case. Although here we start with a $T=0$ scheme the final results can be suitably matched to the finite T description by the proper replacement of the arguments[10].

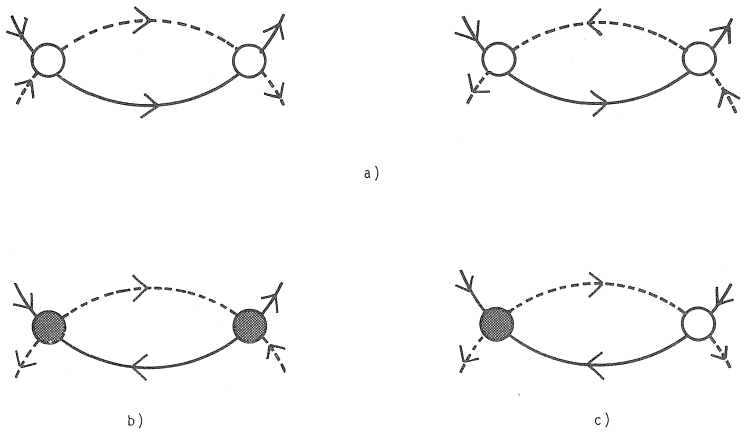


Fig.2. The second order diagrams in the most divergent series.

The first of the most divergent logarithmic contributions comes from the diagrams as shown in Fig.2. If their energy arguments are all of the same order of magnitude such as $\epsilon_i+\xi_i\sim\epsilon_i-\xi_i\sim\omega$, we can find the contributions;

$$\begin{aligned}
&g_1\Gamma_1^{(2a)}(\omega)=g_1^2/(\pi v)\ln(\omega/D),\\
&g_2\Gamma_2^{(2b)}(\omega)=g_1^2/(2\pi v)\ln(\omega/D)-g_3^2/\ln(\omega/D),\\
&g_3\Gamma_3^{(2c)}(\omega)=(g_1-2g_2)g_3/(\pi v)\ln(\omega/D).
\end{aligned} \tag{16}$$

The higher order terms in g in the most divergent series do not make any contribution to the scaling functions because of their dropping out from (9) and the right hand side of (15). All the terms of the form $g^n\ln^{n-1}(\omega/D)$ for $n>2$ are automatically taken into account in the Lie equations. The self energy does not make a contribution in this order, therefore, Ψ_is coincide with Γ_is.

The substitution of (16) into (9) leads to the same results as those by the parquet-diagram sum method[9]. The solutions have unfavorable poles implying the finite temperature phase transition. Thus, the most divergent approach breaks down at temperature corresponding to these poles.

In order to ask for the solutions which are valid over an even lower range of temperature it becomes necessary to go to the next divergent or even lower order series.

The next divergent diagrams of the VF in the third order perturbation are shown in Fig.3. The first of them (Fig.3a), which was calculated by MENYHARD and SOLYOM[8], are composed of only g_1 and g_2 vertices;

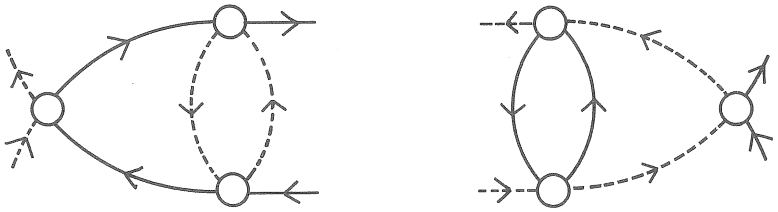


Fig.3. The third order diagrams in the next divergent series.

$$g_1\Gamma_1^{(3a)}(\omega)=2g_1g_2(g_1-g_2)/(2\pi v)^2\ln(\omega/D), \tag{17}$$

$$g_2\Gamma_2^{(3a)}(\omega)=(g_1^3-2g_1^2g_2+2g_1g_2^2-2g_2^3)/(2\pi v)^2\ln(\omega/D).$$

The diagrams containing g_3 vertex are shown in Fig.3b and 3c. Their contributions are;

$$g_1\Gamma_1^{(3b)}(\omega)=-g_1g_3^2/(2\pi v)^2\ln(\omega/D), \tag{18}$$

$$g_2\Gamma_2^{(3b)}(\omega)=(g_2-g_1)g_3^2/(2\pi v)^2\ln(\omega/D),$$

and

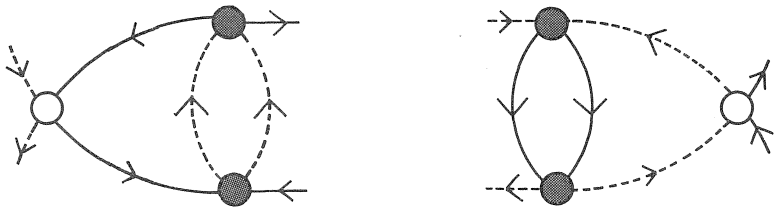


Fig.3b

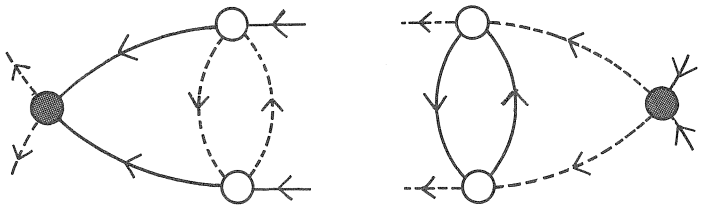


Fig.3c

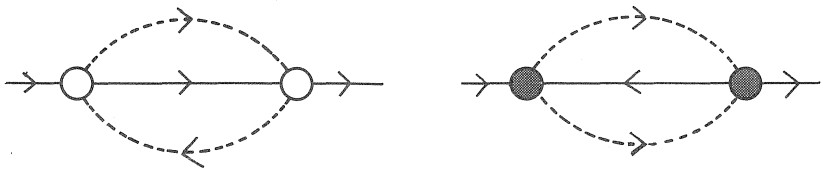
$$g_3\Gamma_3^{(3c)}(\omega)=(g_1-2g_2)g_3/(\pi v)^2\ln(\omega/D). \tag{19}$$

Finally, the electron self-energy as shown in Fig.4 contributes as;

$$\Sigma^{(a)}(p)=(g_1^2-g_1g_2+g_2^2)(\epsilon-\xi_p)/(2\pi v)^2\ln(\omega/D), \tag{20}$$

$$\Sigma^{(b)}(p)=\frac{1}{2}g_3^2/(2\pi v)^2(\epsilon-\xi_p)\ln(\omega/D).$$

The above self-energy contributions are essential to keep the theory so consistent as required by the Ward's identity for VF and GF[8,9,11], and play an important role in canceling many of the vertex contributions in our case.



a) b)

Fig.4. The self-energy diagrams.

§4. The solutions of the Lie equations

Now, it is ready to solve the Lie equations formulated in §2. Incorporating the contributions (16)~(20), and then constructing (9), we obtain from (8) the equations;

$$z\frac{d\Psi_1}{dz}=\Psi_1^2+\frac{1}{2}\Psi_1^3,\qquad z\frac{d\Psi_4}{dz}=\Psi_3^2\left(1+\frac{1}{2}\Psi_4\right),\tag{21}$$

$$z\frac{d\Psi_3}{dz}=\Psi_3\Psi_4\left(1+\frac{1}{4}\Psi_4\right)+\frac{1}{4}\Psi_3^3.$$

where we defined as ; $\Psi_4\equiv\Psi_1-2\Psi_2$.

The solution for the first member of Eq(21) is obtained as ;

$$\ln z=-\frac{1}{\Psi_1}+\frac{1}{2}\ln\frac{\Psi_1+2}{\Psi_1}+\frac{1}{g_1}-\frac{1}{2}\ln\frac{g_1+2}{g_1}.\tag{22}$$

The solutions for Ψ_2 and Ψ_3 cannot be obtained analytically. However, we can see that the monotonous and smooth solutions can be obtained for all Ψ, hence the finite renormalization case I is met in fact for our problem.

In the infrared limit $z\to 0$ in which we are interested Ψ_i tends to the limit λ_i as follows ;

case i) $g_1,\ g_4>0,\ g_3\gtrless 0$; $\lambda_1=\lambda_2=\lambda_3=\lambda_4=0$,

case ii) $g_1,\ g_4<0,\ g_3\gtrless 0$; $\lambda_1=-2,\ \lambda_2=0,\ \lambda_3=\pm 2,\ \lambda_4=-2$,

case iii) $g_1>0,\ g_4<0,\ g_3\gtrless 0$; $\lambda_1=0,\ \lambda_2=1,\ \lambda_3=\pm 2,\ \lambda_4=-2$, (23)

case iv) $g_1<0,\ g_4>0,\ g_3\gtrless 0$; $\lambda_1=-2,\ \lambda_2=-1,\ \lambda_3=\lambda_4=0$.

Following the same procedure as above we find the Lie equations for d and Γ_i from Eqs(14) and (15) as ;

$$z\frac{d}{dz}\ln d(z,g)=\frac{1}{4}(\Psi_1^2-\Psi_1\Psi_2+\Psi_2^2)+\frac{1}{8}\Psi_3^2,\tag{24}$$

$$z\frac{d}{dz}\ln\Gamma_1(z,g)=\Psi_1+\frac{1}{2}(\Psi_1\Psi_2-\Psi_2^2-\frac{1}{2}\Psi_3^2)$$

$$z\frac{d}{dz}\ln\Gamma_2(z,g)=\frac{1}{2\Psi_2}\left\{\Psi_1^2-\Psi_3^2+\frac{1}{2}\Psi_1^3-\Psi_1^2\Psi_2+\Psi_1\Psi_2^2-\Psi_2^3-\frac{1}{2}\Psi_1\Psi_3^2+\frac{1}{2}\Psi_2\Psi_3^2\right\},\tag{25}$$

$$z\frac{d}{dz}\ln\Gamma_3(z,g)=\Psi_1-2\Psi_2-\frac{1}{4}(\Psi_1^2+2\Psi_1\Psi_2-2\Psi_2^2)$$

The asymptotic expressions for d and Γ_i can be readily obtained from Eqs(24) and (25) by using (23) resulting the power type ;

$$d\propto(\omega/D)^{\mu},\qquad \Gamma_i\propto(\omega/D)^{\nu_i}\tag{26}$$

in the neiborhood of zero energy. The power indices μ and ν_i are evaluated as follows ;

case i) $\mu=\nu_i=0$, for $i=1,2,3$,

case ii) $\mu=3/2, \quad \nu_1=-3, \quad \nu_2=0, \quad \nu_3=3,$ (27)

case iii) and iv) $\mu=3/4, \quad \nu_i=-3/2, \quad$ for $i=1,2,3,$

Note that the case iii) involves the Hubbard model: $g_1=g_2=g_3=-g_4>0$.

It is interesting compare these results with those of the case $g_3=0$[8], the case of a partial number of electron per lattice site. The latter can be a also considered by setting $\phi_3=\phi_4\equiv 0$ in Eqs(21) and (25), resulting as;

case v) $g_1>0; \quad \lambda_1=\lambda_2=0, \quad \mu=\nu_i=0, \quad$ for $i=1,2,$

case vi) $g_1<0; \quad \lambda_1=-2, \quad \lambda_2==1, \quad \mu=3/4, \quad \nu_i=-3/2, \quad$ for $i=1,2.$ (28)

Unlike the case $g_3\neq 0$ the limit of the invariant charges and the power indices in (28) are determined solely by the sign on g_1 notwithstanding the sign on g_4.

Finally, we transform these results to the behavior at finite temperature with the help of the matching condition[10]. In doing this we need only notice that the single variable z in Eqs(21) and (25) should be interpreted as T/D provided the characteristic energy ω is of the same order of magnitude as or less than the temperature T. Thus we can conclude that the temperature behaviors of GF and VF are well characterized by

$$d \propto (T/D)^{\mu}, \qquad \Gamma_i \propto (T/D)^{\nu_i}, \tag{29}$$

which are precisely the same power law as (26) and (27).

§ 5. Conclusions and discussions

The investigation of the simple model of 1-D electronic systems with half-filled bands has been developed by means of the renormalization group method, The calculations have been accurate up to the next divergent logarithmic contributions. As a result, the behavior of the invariant charges is always monotonously varying and finite over the entire range of their characteristic energy or of the temperature and free from the ghost poles. Correspondingly, GF and VF obey the power low in energy near the Fermi surface or in temperture near the absolute zero, and the power indices are either equal to zero or of the order of unity with positive (for GF) or negative (for VF) sign. The form of the asymptotic GF and VF is of universal charactor for arbitrary but weak couplings. The divergence in VF has been possible to display exclusively at zero energy and absolute zero temperature. In this point, as in the case of MENYHARD and SOLYOM[8], the present situation makes a fairly striking contrast with the predictions made by DZYALOSHINSKII and LARKIN[9] with the most divergent logarithmic accuracy, where the invariant charges (and VF) displayed unphysical ghost poles. In other words, the present results would predict that phase transitions in our system, if they are possible, should manifest themselves only at the absolut zero temperature, which is in accord with the

HOHENBERG'S theorem[4].

As have been seen from Fig.3, the next divergent graphs involve the density and spin fluctuations accompanied by the electron-hole pair excitations with total momentum$\sim$0 as well as by the electron-electron (hole-hole) pair excitations with total momentum$\sim 2p_F$ (when $g_3=0$). These fluctuations have not played any significant role as long as the invariant charges have remained small as compared with unity. This has been the case if the bare couplings are all positive in sign (case i). However, in the other cases the growing of the invariant charges due to the most divergent contributions has been suppressed by these fluctuations to a large extent, once they have attained the value of or larger than unity. The suppressing effect has been recognized as a general feature underlying the phase transition in 1-D systems.

The perturbation calculations carried out in §3 have shown that if the band is half-filled ($g_3\neq 0$), the umklapp processes as $p_1+p_2=p_3+p_4\pm 4p_F$ make contributions in a logarithmically singular manner to VF and GF. Therefore, as emphasized[9], it was expected that g_3 interaction should strongly affect the properties of the variety of the phases in the present system. Certainly, the infrared-limit of the invariant charges and the power indices of VF and GF have differed in quality from those of the case of $g_3=0$.

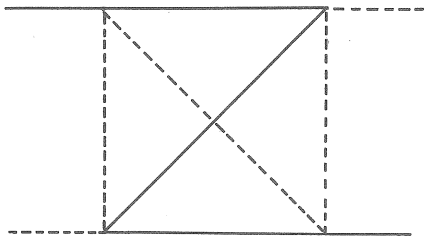


Fig.5. The fourth order diagram in the next-next divergent series.

Strictly speaking, as was recognized in MENYHAD and SOLYOM'S case[8], the present theory is still questionable if the effective expansion parameter of the theory (the invariant charges) becomes comparable with unity. This is actually met in our cases ii)$\sim$iv) as well as in the case vi). Clealy, in principle, any conclusive statement for these cases might be made after the complete account of the whole progressions of the series. Neverthless, our tentative examination of the next-next divergent diagrams as shown in Fig.5 suggests that it dose not significantly alter the present matter of affairs.

The problems that have remained are to predict the observable properties of the systems and also to discuss the possible ordering in the ground states. They will be studied in the author's separate paper.

Acknowledgments

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REFERENCES

1) See for example, M. TAKAHASHI, Prog. Theor. Phys. **44** (1970), 348, **46** (1971), 1388, **47** (1972), 69.
2) J. BARDEEN, Solid State Communications, **13** (1973), 357. P. W. ANDERSON, and M. Saitoh P. A. LEE, ibid. 595.
3) Yu. A. BYCHKOV, L. P. GOR'KOV and I. Ye. DZYALOSHINSKII, Zhur. Eksp. i Teoret. Fiz. **50** (1966), 738.
4) P. C. HOHENBERG, Phys. Rev. **158** (1967), 383.
5) A. WULF and J. F. FERNANDEZ, J. Low Temp. Phys. **7** (1972), 119.
6) M. KIMURA, Prog. Theor. Phys. **49** (1973), 697.
7) See for recent reviews, K.G. WILSON, Phys. Rev. **D3** (1971), 1818 and D. V. SHIRKOV, preprint JINR, E2-7082, Dubna, (1973).
8) N. MENYHARD and J. SOLOM, preprint, Budapest, (1973).
9) I. Ye. DZYALOSHINSKII and A. I. LARKIN, Zhur. Eksp. i Teoret. Fiz. **61** (1971), 791.
10) A. A. ABRIKOSOV and A. A. MIGDAL, J. Low Temp. Phys. **3** (1970), 519.
11) B. ROULET, J. GAVORET and P. NOZIERES, Phys. Rev. **178** (1969), 1079, P. NOZIERES, J. GAVORET and B. ROULET, Phys. Rev. **178** (1969), 1084.