

6-142

ОБЪЕДИНЕННЫЙ ИНСТИТУТ Ядерных Исследований

Дубна

E17-96-142

1996

F.D.Buzatu*

ONE-DIMENSIONAL FERMIONS WITH REPULSIVE DELTA-FUNCTION INTERACTION IN THE BRUECKNER THEORY

Submitted to «Physical Review B»

*E-mail: buzatu@thsun1.jinr.dubna.su Permanent address: Department of Theoretical Physics, Institute of Atomic Physics, Magurele — Bucharest MG-6, Romania

1) Introduction. It is well known that the Landau quasi-particle description of the Fermi liquids breaks down in one dimension (1D) [1]. An alternative theory, based on an exactly soluble model [2], leads to the concept of the Luttinger liquid [3], with distinct properties [4]. Nevertheless, a clear explanation for the failure of the usual Fermi liquid behavior and a physical picture of the salient features of the system are, in our opinion, still missing. It is the aim of this paper to put forward such a picture, using a well-known method introduced in nuclear physics many years ago in order to overcome the difficulties associated with the hard-core interactions: the Brueckner theory (BT) [5]. We shall apply here the Brueckner and Gammel (BG) method [6] to determine self-consistently the single-particle energies (SPE) and the ground-state energy (GSE) for the 1D repulsive delta model (RDM), i.e. a system of fermions interacting via a repulsive δ -function potential, its Bethe-Ansatz (BA) solution [7] providing a good test to check our considerations.

2) The model. The Hamiltonian for the 1D RDM in the second quantization (momentum representation) reads aksa tabah Mathiling mpi na da dagar le dentar ne dentar kembara ang katakan katakan

$$\mathcal{H} = \sum_{k,\sigma} \varepsilon_0(k) c^{\dagger}_{k,\sigma} c_{k,\sigma} + C \sum_{k_1 - 3,\sigma,\sigma'} c^{\dagger}_{k_1 + k_3,\sigma} c^{\dagger}_{k_2 - k_3,\sigma'} c_{k_2,\sigma'} c_{k_1,\sigma}$$
(1)

where, in the chosen units, rol

14. T. . . . lo sine si

$$\varepsilon_0(k) = k^2_{(1)}, \quad k \in (-\infty, +\infty)$$

is the SPE of the noninteracting fermions, C > 0 is the (dimensionless) coupling constant and $c^{\dagger}(c)_{k,\sigma}$ denotes the usual Fermi creation (annihilation) operator of a one-particle state with a given momentum k (in units of the Fermi momentum k_F) and spin $\sigma = \pm 1/2$. It was assumed in (1) that the system is enclosed in a large box of finite length but we shall consider in fact only the thermodynamic limit. In the BA approach, the GSE of the 1D RDM can be found by solving an integral equation; the numerical results [8] have been compared with other approximate schemes, the T-matrix approximation (TMA) [9] giving the best agreement with the BA solution.

to give allocidally harded. In the south wells, where is a degrade is sent index stated (Adapted a) story chilence was left in philes the state of the builty an elements for a second se and which have been been deal appendix of the and the deal and the second states of the second states and the set platter and put interfaces in any party of a realistic of the build a section of



3) The method. The idea of the BT can be easily understood by comparing it with the Hartree-Fock method [10, 11]: if the last one considers the motion of a particle in the average field produced by the others (independentparticle approximation), in the Brueckner's approach the interaction of any two particles is treated exactly and the effect of the rest of the particles on the interacting pair is replaced by an average (independent-pair approximation). According to the BT, the effective interaction between two particles is described by the reaction matrix K, solution of an integral equation depending on the bare potential and on the still undetermined SPE [12]; these energies are assumed to have the Hartree-Fock form, with the one-particle potential given by the diagonal elements of the K-matrix. Formally, the problem reduces to find a solution for the SPE from these two coupled equations; however, while there is a unique prescription to calculate the energy ε of a particle in the ground state, the energy ϵ of a particle in an excited state cannot be uniquely defined and this is a major difficulty in the BT. Let us consider a pair of particles having the ground state momenta l and l', respectively (|l|, |l'| < 1); such a state can be understood as a result of all the possible virtual scatterings of the two particles in the excited states: $\{l, l'\} \rightarrow \{h, h'\} \rightarrow \{l, l'\}$ (|h|, |h'| > 1). Let us denote by W the starting energy [13], i.e. the sum of the hole energies minus the sum of the particle energies, except the pair under consideration, in a given configuration; when W coincides with the total energy $\Omega = \varepsilon(l) + \varepsilon(l')$ of the initial (final) two-particle state, we say that the K-matrix is calculated on-energy-shell (OnES), otherwise K is said to be calculated off-energy-shell (OffES). In the process considered above, the energy $\varepsilon(l)$ is expressed in, terms of K[W] computed OnES, i.e. with $W = \Omega$; in the integral equation corresponding to this K-matrix occur also the undefined energies $\epsilon(h; h', \Omega)$ and $\epsilon(h'; h, \Omega)$, depending on the actual configuration of the particles. ϵ can be in principle determined from another K-matrix computed OffES; this new K-matrix obeys an integral equation similar to the first one but demanding the knowledge of an ϵ with a more complicated history, and so on endless. BG [6] neglected the dependence of ϵ on the history and they replaced it by $\epsilon(h; \Omega - \Lambda)$, where Λ is a parameter denoting an average excitation energy for a particle (it will be discussed below). Consequently, the propagation in the virtual excited states will depend parametrically only on the total energy Ω of the initial two-particle state (also on Λ , but it enters as a parameter in the whole calculation of both ϵ and ϵ , a dependence which will be not explicitly specified). The OffES propagation can be determined by solving at first the corresponding K-matrix equation in terms of ϵ and then by finding ϵ from the resulting integral equation given by its Hartee-Fock form. The spectrum of the virtual excitations is used after that to determine the OnES propagation, i.e. the energy ε of an unexcited state.

2. 2. 3. 3 . 4. 3 . 4.

等于在不可能。这些说:"是不是我的教育。

4) The equations for the single-particle energies. In the particular case of a constant interaction in the k-space, the K-matrix equation solves immediately independent on the SPE form. The resulting integral equations for ε and ϵ corresponding to the 1D RDM in the BG method are:

$$\left(\begin{array}{c} \varepsilon(l) = \varepsilon_0(l) + V(l) \\ \end{array} \right), |l| < 1$$
(3)

$$\left(\epsilon(h;\Omega) = \varepsilon_0(h) + \mathcal{V}(h;\Omega) , |h| > 1 \right)$$

where the one-particle potentials V and V are given by

$$\begin{cases} V(l) = \frac{C}{\pi} \int_{-1}^{1} \left[1 + \frac{C}{\pi} \int_{\mathcal{D}_{K}} \frac{dq}{e(q;l,l')} \right]^{-1} dl' , K = l + l' \\ V(h;\Omega) = \frac{C}{\pi} \int_{|K|<2}^{1} \left[1 + \frac{C}{\pi} \int_{\mathcal{D}_{K}} \frac{dq}{e(q;K,\Omega)} \right]^{-1} dl , K = l + h \end{cases}$$
(4)

with the notations

$$\begin{cases} e(q; l, l') = \epsilon[K/2 + q; \Omega(l, l')] + \epsilon[K/2 - q; \Omega(l, l')] - \Omega(l, l') \\ e(q; K, \Omega) = \epsilon(K/2 + q; \Omega) + \epsilon(K/2 - q; \Omega) - \Omega + \Lambda \end{cases}$$
(5)
In the first (second) line of Eq. (5) $K = l + l'$ ($K = h + l$) and
$$\begin{cases} \Omega(l, l') = \epsilon(l) + \epsilon(l') \\ \Omega \in [2\epsilon(0), 2\epsilon(1)] \end{cases}$$
(6)

The range \mathcal{D}_{K} in the second integrals from Eqs. (4), defined by

$$\mathcal{D}_{K} = (-\infty, -|K|/2 - 1) \cup (|K|/2 + 1, +\infty)$$
(7)

and consistent with the form of the denominators (5), restricts all the intermediate scatterings to the states above the Fermi level. The definition (7) is a consequence of two requirements: (i) only the principal part of the q-integrals (in general, over all possible values of q) has to be taken [5]; (ii) the exclusion principle is satisfied in the intermediate unexcited states [10]. However, let us note that the definition (7) follows from (i) and (ii) only if all the energies of the excited states are higher than those of the unexcited ones, an implicit assumption for a normal Fermi liquid.

3

5) The average excitation energy. The parameter Λ has been introduced as an average excitation energy of a particle. In the nuclear matter calculations it was considered an arbitrary quantity taking values from 0 to $\varepsilon(1)-\varepsilon(0)$ corresponding to the energy difference of particles lying respectively at the top and the bottom of the Fermi sea; the results depend only weakly on the values of Λ [6] justifying, in the BG opinion, the introduced approximations. Let us note that the above range of Λ implicitly assumes that there is no gap at the Fermi level between the OnES and OffES propagations (in fact it occurs for the nuclear matter [14]); by allowing such a possibility, we should define the range as:

$$\Lambda \in [\epsilon(1;\Omega_{max}) - \varepsilon(1), \epsilon(1;\Omega_{max}) - \varepsilon(0)]$$
(8)

where Ω_{max} denotes the maximum value of Ω (we shall use also Ω_{min} with a similar meaning). However, the definition of Λ is still ambiguous: the limits of the range (8) depend themselves on the initial value of Λ used in the determination of ε and ϵ . In a full self-consistent treatment Λ should be uniquely determined from its definition; this can be done by averaging the momentum dependence of ε . We defined Λ as the arithmetical mean of the two limits of its range (8):

$$\Lambda = \epsilon \left(1; \Omega_{max}\right) - \frac{1}{2} \left[\varepsilon(0) + \varepsilon(1)\right]$$
(9)

This choice corresponds to a minimum average excitation energy (assuming ε a convex function of its variable, as it follows from the numerical computations). The condition (9) determines self-consistently the parameter Λ .

6) Numerical results. The integral coupled equations (3) can be solved numerically by iteration, starting with the free expression (2) for the SPE and with $\Lambda = 0$; the first iteration results (TMA) in the $C = \infty$ case are represented in Fig. 1 by dashed lines. For the OffES propagation only two curves have been drawn: the lower (upper) one corresponds to $\Omega = \Omega_{max}$ (Ω_{min}). For $k \geq 3$ the OffES curves join the free dispersion law $\varepsilon_0(k)$, a consequence of the assumption that in the intermediate states |K| < 2. The same property occurred in the BG results for $|\vec{k}| \geq 2.6k_F$ [6] and reflects the fact that the excitations with the momentum far from the Fermi level obey the same dispersion law as in the free case. But a more important remark is the discontinuity at the Fermi momentum (1 in our units) between $\varepsilon(1)$ and $\epsilon(1;\Omega_{max})$ corresponding to a negative gap (NG) and not to a positive one as in the nuclear matter calculations [14]. We could try to avoid the occurrence of such a NG at each iteration step by increasing the value of Λ ; the convergency is reached after a few iterations, but the value of Λ required to vanish the NG will be much greater (at least for strong couplings) than the value indicated by the right side of Eq. (9). It follows that the NG is unavoidable. As a result, the denominators e given by Eqs. (5) will vanish for some values of the q-variable, contradicting thus the condition (i) mentioned above. Consequently, only the principal part of the q-integrals from Eqs. (4) must be taken; in our case, the definition (7) of the range \mathcal{D}_{K} does not guarantee this fact. The self-consistent solution of the system (3) and (9), i.e. in the K-matrix approximation (KMA), corresponds for $C = \infty$ to $\Lambda = 0$; the results for the SPE are represented in Fig. 1 by continuous lines. The final value Δ of the NG is approximately -0.6. For smaller values of the interaction constant C, both ε and ϵ get closer to the free dispersion law ε_0 , concomitantly with a reduction of the NG and an increase of Λ ; in the $C \to 0$ limit, $\Delta \to 0$ and $\Lambda \to 0.5$. From the results presented in Fig. 1 it follows also that the main effect of the interaction on the OnES propagation is to shift the values of ε_0 by a constant quantity, i.e. the average potential V experienced by a fermion in the ground-state depends very weak on its momentum (see Fig. 2); this is of course a consequence of the k-independence of the bare potential in the momentum representation. 7) The effective potential picture. The occurrence of a NG at the Fermi surface, a consequence of the kinetic restrictions imposed by the momentum conservation on the two-body scatterings, signals the breakdown of the usual quasi-particle picture in 1D: it is related, through the diagonal elements of the reaction matrix entering in the calculation of the SPE, with a singular forward scattering of two particles [1]. The NG determines an instability of the Fermi surface, the particles close to it looking for more stable positions. This fact can be interpreted as follows. Let'us consider two particles from the top of the unstable Fermi surface, with the total energy Ω_{max} . According to the KMA results, their lowest "excited" states correspond to the bottom of the OffES region from Fig. 1 and the two particles have the tendency to occupy these positions because they are less energetic than the initial ones; the final energy of the pair would be $2\epsilon(1;\Omega_{max}) < \Omega_{max}$ in such a case. However, by decreasing its energy, the pair will be excited along a curve above the lowest one, corresponding to an $\Omega < \Omega_{max}$; it can be considered as stable when its final energy Ω_{lim} equals the total energy of the partners in their lowest excited

$$\Omega_{lim} = 2\epsilon \left(1; \Omega_{lim}\right) \tag{10}$$

a condition that determines Ω_{lim} . Consequently, the highest OnES state will go down from $\varepsilon(1)$ level to $\Omega_{lim}/2$ at the same value of the momentum. Something similar happens with the rest of the particles which will lose energy not only due to their unstable positions but also as an effect of the particles already fallen down (the effective repulsion between the particles decreases). In other words, we introduce an effective one-particle potential V_{eff} , instead of the original

5

states (no NG), i.e. when

one V, describing the rearrangement of the particles induced by the occurrence of the NG. In the |l| = 1 limit, the OnES potential V_{eff} is determined by the condition (10) of continuity with the OffES one \mathcal{V} at the Fermi level; we can define it for |l| < 1 as the shifted values of V with the same quantity as for |l| = 1, i.e. by

$$V_{eff}(l) = V(l) - \Delta V \quad , \quad \Delta V = (\Omega_{max} - \Omega_{lim})/2 \tag{11}$$

an assumption justified by the weak dependence of the original one-particle potential V on the momentum. The one-particle potentials, both OnES and OffES (only the delimiting curves), in this effective potential picture (EPP) are represented in Fig. 2 by dashed lines, where the same quantities in the KMA are drawn by continuous lines. The role of the effective one-particle potential introduced above is to simulate a normal Fermi liquid behavior in the presence of the instability determined by the NG at the Fermi level; V_{eff} should be considered merely as a convenient tool to compute some quantities, such as the GSE. In discussing the nature of the lowest-energy excitations, the fact that the particles close to the Fermi level are unstable to transitions in states with a higher momentum has important consequences; a possible picture in this sense is given below.

8) The fermion-boson picture. We give now another interpretation of the instability induced by the occurrence of the NG at the original Fermi surface. We shall assume that beginning from the top of the unstable Fermi sea, the particles will fall down on their lowest energetic positions from the excitation spectrum (corresponding to $k = \pm 1$). This process ends when the level of the remaining Fermi sea is as high as the upper level of the filled vertical edges at the Fermi momentum (see Fig. 3), i.e. when the same condition (10), but with

$$\Omega_{lim} = 2\varepsilon (k_F^{eff}) \tag{12}$$

is fulfilled; we have defined in this way an effective Fermi momentum k_F^{eff} . The particles at $k = \pm 1$ can be viewed either as fermions, if one employs an Ω -type label for their states, or as bosons, in the momentum representation; they can be considered as an 1D effect induced by the necessity of taking into account diagrams in the linked cluster expansion contradicting the exclusion principle [11, 13]. The emerging ground-state configuration in this fermion-boson picture (FBP) [15] consists thus of a reduced sea of core fermions for $|k| < k_F^{eff}$ and a certain number of shell bosons at $k = \pm 1$ that are essential in describing the excitations of the system. 9) The ground-state energy. In the BT, the GSE is computed from

$$E = \frac{1}{\pi} \int_{-1}^{1} \left[\varepsilon_0(l) + \frac{1}{2} V(l) \right] dl = \frac{2}{3\pi} + \frac{1}{\pi} \int_{0}^{1} V(l) dl$$
(13)

where E represents the density of the GSE in units of $k_{\rm F} \epsilon_0(k_{\rm F})$. The values of E for $C \leq 6$ in TMA are along the dashed line from Fig. 4; they coincide with the results obtained previously [9]. The maximum (relative) deviation from the BA values [8] is realized when $C = \infty$: it decreases from 20 % in the TMA to 9 % in the KMA (without taking into account the NG problem). The GSE in the EPP is determined from the same Eq. (13) but with V_{eff} instead of V. In calculating the GSE in the FBP, we divided the last integral from Eq. (13) in two parts: from 0 to k_F^{eff} , computed by using the KMA results for V, and from k_F^{eff} to 1. The contribution of the second term was assumed to depend on a parameter $t \in [0, 1]$ describing the continuous transformation from $\{l, V(l)\}$ at t = 0 to $\{1, V[1; 2\varepsilon(l)]\}$ at t = 1; the range $[k_F^{eff}, 1]$ is mapped for any $t \neq 1$ in another one $[\kappa_t, 1]$, with $\kappa_0 = k_F^{eff}$ and $\lim_{t \to 1} \kappa_t = 1$, while the transformed values of V(l) are finite at any t. It follows that the second term goes to zero, i.e. the contribution of the shell bosons to the GSE is the same as that corresponding to the free particles above the k_F^{eff} -level. The results in the $C = \infty$ case are: E = 0.856 in the EPP and E = 0.489 in the FBP (with $k_F^{eff} = 0.876$), while the BA value is $E = 8/(3\pi)$, i.e. a relative deviation less than 1 % in the EPP and practically a numerical coincidence in the FBP. For $C \leq 6$, the values of E in the KMA, EPP and FBP are very close to each other (in the weak coupling regime, the NG problem becomes irrelevant for the GSE); the results in the FBP are along the continuous curve from Fig. 4 and they cannot be distinguished from the BA values at the figure scale.

10) Final remarks. Within the FBP, the lowest-energy excitations starting from the interacting ground-state correspond to those of the shell bosons: a spin exchange between them across the two edges gives rise to a $2k_F$ -spin density wave and a similar transfer of a boson (with spin 0 and momentum $2k_F$) corresponds to a $4k_F$ -charge density wave, indicating the *charge-spin* separation that occurs in 1D systems. A detailed discussion of the excitation spectrum will be given elsewhere.

In solving the integral equations for the SPE, it was assumed the existence of the same Fermi momentum k_F in the interacting case as for the free system; the results indicate the occurrence of a NG at this value of the momentum and thus an instability of the original Fermi level. Both the EPP and FBP are *a posteriori* interpretations of this result which clearly shows that one cannot have a ground-state configuration of the interacting particles as in the free case (two particles per k between $-k_F$ and $+k_F$). In the EPP such a

- E **7**,

And the second second



Figure 1: The SPE versus the momentum (in units of k_F) for the 1D RDM with an infinite coupling constant C in the TMA and KMA.



Figure 2: The one-particle potentials versus the momentum for the 1D RDM with an infinite coupling constant C in the KMA and EPP.

Sec.



Figure 3: The ground-state configuration for the 1D RDM in the FBP (schematic representation).



Figure 4: The GSE of the 1D RDM in the TMA and FBP as function of the interaction constant.

normal Fermi liquid configuration was simulated by an effective single-particle spectrum. In the FBP we assumed a redistribution of the unstable particles in accordance with the KMA results and we obtained a picture close to the usual interpretation from the bosonization theory. However, there is in principle another possible way to tackle the problem : one can introduce a priori in the BG equations for the SPE a certain occupancy ρ of a k-state, the conservation of the total number of particles defining thus a new Fermi momentum; ρ could be determined at any iteration step (starting with $\rho = 2$) from the condition of no gap between OnES and OffES propagations. A self-consistent solution with $\rho < 2$ is expected; the analogy with the BA results suggests, in the $C = \infty$ case, $\rho = 1$ and $\varepsilon = \varepsilon_0$. This approach will be discussed in detail in a forthcoming paper.

The occurrence of a NG in the excitation spectrum of a Fermi liquid with pure repulsive interactions is, in our opinion, strictly related to the dimensionality of the system; it has been also found in the 1D Hubbard model [16]. The existence of such a gap could be relevant in the dispute about a possible breakdown of the usual Fermi liquid behavior in 2D.

In conclusion, one might say that the BA results for the GSE of a 1D system of fermions interacting through a repulsive δ -potential can be reproduced within the approximate BG method with a certain, natural self-consistency condition imposed on the parameter Λ of this theory and interpreting, in an appropriate manner, the instability induced by the occurrence of the NG at the Fermi level. One might have expected perhaps such a result, as the system under consideration is an extremely dilute Fermi liquid (short-range correlations); it remains as interesting to apply the BT to an exactly solved model with a long-range interaction. In addition, this independent-pair approximation suggests some possible connections with well known results from the BA and bosonization theory.

Acknowledgments

The author is grateful to M. Apostol, V.I. Inozemtsev, F. Mancini, D. Villani and J. Voit for helpful suggestions, critical remarks and stimulating discussions related to this subject.

10

References

- The breakdown of the Landau's Fermi liquid theory in 1D is signaled by a singular forward scattering: P.W. Anderson, Phys. Rev. Lett. 64, 1839 (1990); 65, 2306 (1990); see also P.W. Anderson and D. Khveshchenko, Phys. Rev. B 52, 16415 (1995).
- [2] J.M. Luttinger, J. Math. Phys. 4, 1154 (1963); D.C. Mattis and E.H. Lieb, J. Math. Phys. 6, 304 (1965).
- [3] F.D.M. Haldane, J. Phys. C 14, 2585 (1981).
- [4] For a recent review on the Luttinger liquid properties see, for example, J. Voit, Rep. Prog. Phys. 58, 977 (1995).
- [5] K.A. Brueckner and C.A. Levinson, Phys. Rev. 97, 1344 (1955); K.A. Brueckner, Phys. Rev. 100, 36 (1955); see also Refs. [10, 11] below.
- [6] K.A. Brueckner and J.L. Gammel, Phys. Rev. 109, 1023 (1958).
- [7] M. Gaudin, Phys. Lett. A 24, 55 (1967); C.N. Yang, Phys. Rev. Lett. 19, 1312 (1967).
- [8] W.I. Friesen and B. Bergersen, J. Phys. C 13, 6627 (1980).
- [9] S. Nagano and K.S. Singwi, Phys. Rev. B 27, 6732 (1983).
- [10] H.A. Bethe, Phys. Rev. 103, 1353 (1956).
- [11] J. Goldstone, Proc. Roy. Soc. (London) A 239, 267 (1957).
- [12] In our terminology, the T-matrix corresponds to the solution of the same integral equation but with the self-consistent single-particle energies replaced by the kinetic energies.
- [13] B.D. Day, Rev. Mod. Phys. 39, 719 (1967).
- [14] K.A. Brueckner and D.T. Goldman, Phys. Rev. 117, 207 (1960).
- [15] A fermion-boson duality has been previously emphasized in: M. Apostol,
 V. Bârsan and C. Mantea, Rev. Roum. Phys. 29, 673 (1984).

[16] F.D. Buzatu, R. Hayn and V. Oudovenko, in preparation.

Received by Publishing Department on April 22, 1996.