## **Exact Bosonization for an Interacting Fermi Gas in Arbitrary Dimensions**

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We present an exact mapping of models of interacting fermions onto boson models. The bosons correspond to collective excitations in the initial fermionic models. This bosonization is applicable in any dimension and for any interaction between fermions. Introducing superfields, we derive a field theory that may serve as a new way of analytical study. We show schematically how the mapping can be used for Monte Carlo calculations and argue that it should be free from the sign problem.

DOI: 10.1103/PhysRevLett.103.186403

PACS numbers: 71.10.Ay, 71.10.Pm, 75.40.Cx

The study of interacting fermionic systems in cases when the Landau Fermi liquid theory fails to describe all interesting effects is an open problem of condensed matter theory. Very often conventional methods [1] are not efficient due to divergencies in perturbation expansions leading to the resummation of complicated series.

It is difficult to list here all the problems encountered in the study of, e.g., strongly correlated systems. The most clear examples are provided by one dimensional (1D) systems where perturbative methods are especially inconvenient but models suggested for describing high  $T_c$  superconductivity, see, e.g. [2], are not simpler. Generically, the low temperature physics of systems of interacting fermions is naturally described in terms of bosonic collective excitations that can be expressed only by an infinite series of conventional diagrams.

The numerical study of fermionic systems encounters difficulties as well. The powerful Monte Carlo (MC) method suffers the well-known sign problem [3–7] leading to a drastic increase in the computing time.

All these examples call for a reformulation of interacting fermions in terms of a boson model. Such an approach, called bosonization (see, e.g., [8,9]), is well known and successful for 1D fermionic systems. Attempts to bosonize fermionic models in the dimensionality d > 1 have been undertaken in the past, starting from the works [10,11] followed by [12]. These schemes, however, have problems when dealing with large momentum transfer by the interaction [13]. They reproduce the random phase approximation (RPA) but do not reach beyond.

A more general low energy bosonization scheme suggested recently [14] is based on quasiclassical equations and takes into account large momentum transfer. New logarithmic contributions to anomalous dependence of the specific heat [14] and spin susceptibility [15] were found. However, working well for d = 1 the scheme of Ref. [14] is not completely accurate for d > 1 missing some effects of the Fermi surface curvature [16].

All the previous bosonization methods are not exact; hence they cannot be used for accurate numerical studies of the initial fermionic problem. In this Letter, we present a new scheme that allows one to map interacting fermions to interacting bosons *exactly*. This mapping works in any dimension at any temperature. The effective model obtained describes interacting bosonic excitations. It can be written either in a form of a model of noninteracting bosons in a Hubbard-Stratonovich (HS) field with a subsequent integration over this field or in a form of a field theory containing superfields with quartic and cubic interactions. The former may be convenient for MC study, while the latter promises to be good for analytical investigations.

We start with a general model of interacting electrons described by the Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}},\tag{1}$$

where  $\hat{H}_0$  is the bare part,

$$\hat{H}_0 = -\sum_{r,r',\sigma} t_{r,r'} c^+_{r\sigma} c_{r'\sigma} - \mu \sum_{r,\sigma} c^+_{r\sigma} c_{r\sigma}, \qquad (2)$$

and  $\hat{H}_{int}$  stands for an electron-electron interaction,

$$\hat{H}_{\text{int}} = \frac{1}{2} \sum_{r,r'\sigma,\sigma'} V_{r,r'} c^+_{r\sigma} c^+_{r'\sigma'} c_{r'\sigma'} c_{r\sigma}.$$
 (3)

In Eqs. (1)–(3)  $c_{r\sigma}$  ( $c_{r\sigma}^+$ ) are annihilation (creation) operators of the electrons on a lattice site *r* with spin  $\sigma = \pm$ . The function  $t_{r,r'}$  describes the tunneling from the site *r* to the site *r'*,  $V_{r,r'}$  is the electron-electron interaction between the *r* and *r'* and  $\mu$  is the chemical potential.

The scheme of the bosonization suggested here can be developed for arbitrary functions  $t_{rr'}$  and  $V_{rr'}$  in an arbitrary dimension. However, in order to make formulas more compact we assume that

$$V_{r,r'} = \delta_{r,r'} V_0, \qquad V_0 > 0, \tag{4}$$

which corresponds to an on site repulsion.

Then, the term  $\hat{H}_{int}$  can be rewritten in the form

$$\hat{H}_{\text{int}}^{(0)} = -\frac{V_0}{2} \sum_{r} (c_{r,+}^+ c_{r,+} - c_{r,-}^+ c_{r,-})^2$$
(5)

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while replacing the chemical potential  $\mu$  by  $\mu' = \mu - V_0/2$ .

In this Letter, we concentrate on studying thermodynamics and calculate the partition function

$$Z = \text{Tr} \exp(-\beta \hat{H}), \qquad \beta = 1/T.$$
 (6)

As  $\hat{H}_0$  and  $H_{\text{int}}^{(0)}$  do not commute we subdivide the interval  $(0, \beta)$  into slices of the length  $\Delta = \beta/N \ll \beta$  and write Z as a time ordered product over the imaginary time  $\tau$ . Following a standard route of the HS transformation we decouple the interaction term  $\hat{H}_{\text{int}}^{(0)}$  integrating over a periodic real field  $\phi_r(\tau) = \phi_r(\tau + \beta)$  and come to

$$Z = \lim_{\Delta \to 0} \int Z[\phi] \exp\left[-\frac{\Delta}{2V_0} \sum_{r} \sum_{l=1}^{N} \phi_{r,l}^2\right] D\phi,$$

$$Z[\phi] = \operatorname{Tr}\left[\exp\left(-\frac{\hat{H}_0}{T}\right) \prod_{l=1}^{N} \exp\left(\Delta \sum_{r,\sigma} \sigma \phi_{r,l} \bar{c}_{r,\sigma,l} c_{r,\sigma,l}\right)\right],$$
(7)

 $c_{r,\sigma,l}$  and  $\bar{c}_{r,\sigma,l}$  are the annihilation and creation operators in the interaction representation [1] taken at  $\tau_l = (l-1/2)\Delta$ ,  $D\phi$  is the normalized product of all differentials  $d\phi_{r,l}$  and  $\phi_{r,l} = \phi_r(\tau_l)$ . The product in  $Z[\phi]$  is ordered in time, such that l = 1 is on the right.

For the analytical study, we could write Eq. (7) explicitly in the continuous limit  $\Delta \rightarrow 0$  using integrals and time ordering operators  $T_{\tau}$ . However, MC calculations imply finite  $\Delta$  with typical values of  $\phi_{r,l}$  growing as  $\Delta^{-1/2}$  for  $\Delta \rightarrow 0$  and therefore, we keep finite  $\Delta$ .

Calculation of the trace over the fermionic operators in Eq. (7) is not simple for finite  $\Delta$  and one should approximate  $Z[\phi]$  by a more convenient expression. A standard approximation  $Z_f[\phi]$  used in MC simulations instead of  $Z[\phi]$ , Eq. (7), reads [3,6]

$$Z_{f}[\phi] = \det_{r,\sigma} \left[ 1 + \prod_{l=1}^{N} \exp(-\hat{h}[\phi(\tau_{l})]\Delta) \right], \qquad (8)$$
$$\hat{h}_{r,\sigma}[\phi(\tau)] = \hat{\varepsilon}_{r} - \mu' - \sigma\phi_{r}(\tau)$$

where  $\hat{\varepsilon}_r f_r \equiv -\sum_{r'} t_{r,r'} f_{r'}$  for an arbitrary function  $f_r$ .

We suggest here another approximation  $Z_b[\phi]$  to  $Z[\phi]$  that is more suitable for the bosonization,

$$Z_{b}[\phi] = \operatorname{Tr}\left[\exp\left(-\frac{\hat{H}_{0}}{T}\right)T_{\tau} \times \exp\left(\sum_{r,\sigma}\int_{0}^{\beta}\sigma\tilde{\phi}_{r}(\tau)\bar{c}_{r,\sigma}(\tau)c_{r,\sigma}(\tau)d\tau\right)\right], \qquad (9)$$
$$\tilde{\phi}_{r}(\tau) = \phi_{r,l} \quad \text{for} \quad (l-1)\Delta \leq \tau < l\Delta.$$

The functional  $Z_b[\phi]$ , Eq. (9), differs from  $Z[\phi]$ , Eq. (7), by integration of the operator  $\bar{c}_{r,\sigma}(\tau)c_{r,\sigma}(\tau)$  over each slice instead of taking it in the middle of the slice and multiplying by  $\Delta$ . Therefore, the difference between  $Z_b[\phi]$  and  $Z[\phi]$  should vanish in the limit  $\Delta \rightarrow 0$ . The functional  $Z_b[\phi]$ , Eq. (9), has a form of the exact partition function for an electron in an external (generally, discontinuous in time) field  $\tilde{\phi}_r(\tau)$  and we can use standard transformations.

In order to reduce the fermionic model, Eq. (9), to a bosonic one, we introduce as in Ref. [14] an additional variable  $0 \le u \le 1$  and write the function  $Z_b[\phi]$  as

$$Z_b[\phi] = Z_0 \exp\left[\sum_{r,\sigma} \int_0^\beta \int_0^1 \sigma \tilde{\phi}_r(\tau) G_{r,r;\sigma}^{(u\phi)}(\tau,\tau+0) du d\tau\right]$$

where  $Z_0$  is the partition function of the ideal Fermi gas and  $G_{r,r';\sigma}^{(u\phi)}(\tau, \tau')$  is a fermionic Green function,

$$\left(-\frac{\partial}{\partial\tau} - \hat{h}_{r,\sigma}[u\tilde{\phi}(\tau)]\right) G^{(u\phi)}_{r,r';\sigma}(\tau,\tau') = \delta_{r,r'}\delta(\tau-\tau'), \quad (10)$$

with the boundary conditions

$$G_{r,r';\sigma}^{(u\phi)}(\tau,\tau') = -G_{r,r';\sigma}^{(u\phi)}(\tau+\beta,\tau') = -G_{r,r';\sigma}^{(u\phi)}(\tau,\tau'+\beta).$$

We develop our bosonization scheme introducing

$$A_{r,r'}(z) = G_{r,r'}^{(0)}(\tau, \tau+0) - G_{r,r';\sigma}^{(u\phi)}(\tau, \tau+0),$$
(11)

where  $z = (\tau, \sigma, u)$  and  $G_{r,r'}^{(0)}(\tau, \tau')$  is the bare electron Green function. The function  $A_{r,r'}(\tau)$  is periodic,  $A_{r,r'}(\tau) = A_{r,r'}(\tau + \beta)$ , and, hence, describes bosons.

We rewrite the partition function  $Z[\phi]$  as

$$Z_b[\phi] = Z_0 \exp\left[-\sum_{r,\sigma} \int_0^\beta \int_0^1 \sigma \tilde{\phi}_r(\tau) A_{r,r}(z) du d\tau\right], \quad (12)$$

and derive a closed equation for  $A_{r,r'}(z)$ . For that purpose we write a conjugated equation

$$\left(\frac{\partial}{\partial \tau'} - \hat{h}_{r',\sigma}[u\tilde{\phi}(\tau')]\right) G^{(u\phi)}_{r,r';\sigma}(\tau,\tau') = \delta_{r,r'}\delta(\tau-\tau')$$

and subtract it from Eq. (10) putting in the resulting equation  $\tau' = \tau + 0$ . The same can be done for the bare Green function  $G_{r,r',\sigma}^{(0)}(\tau, \tau')$  and finally we obtain

$$\frac{\partial}{\partial \tau} A_{r,r'}(z) + \mathcal{H}_{r,r'}(z) A_{r,r'}(z) = -u\sigma \tilde{\Phi}_{r,r'}(\tau) n_{r,r'},$$
$$\mathcal{H}_{r,r'}(z) = \hat{\varepsilon}_r - \hat{\varepsilon}_{r'} - u\sigma \tilde{\Phi}_{r,r'}(\tau),$$
$$\tilde{\Phi}_{r,r'}(\tau) = \tilde{\phi}_r(\tau) - \tilde{\phi}_{r'}(\tau).$$
(13)

The function  $n_{r,r'} = G_{r,r'}^{(0)}(\tau, \tau + 0)$  in Eq. (13) is the Fourier transform in r - r' of the Fermi distribution. Equation (13) should be supplemented by the condition

$$\sum_{r} A_{r,r}(z) = 0.$$
(14)

Equation (14) can be obtained noticing that  $\sum_{r} A_{r,r}(z)$  is a constant independent of  $\phi_r(\tau)$ , which follows from Eq. (13). Assuming that the interaction and, hence,  $\phi_r(\tau)$  vanishes at infinity we come to Eq. (14).

So, we are to solve the linear equation (13) for  $A_{r,r'}(z)$  with the condition (14), substitute the solution into Eq. (12) and then into the first equation (7). A possible strong

discontinuity of the function  $\tilde{\phi}$  does not lead to any problems in the limit  $\Delta \rightarrow 0$ . Our scheme is similar to that of Ref. [14] developed in the quasiclassical approximation but now all the transformations are exact.

It is convenient to exactly integrate over the field  $\phi_r(\tau)$  in the beginning and thus derive a field theory for interacting bosons. In Ref. [14] this goal has been achieved by integrating over 48-component supervectors, which has led to a rather cumbersome Lagrangian. Now we use another trick, known as the Becchi-Rouet-Stora-Tuytin (BRST) transformation, based on introducing superfields [17] (see also the book [18]). A similar transformation was used in the quantization of non-Abelian gauge theories [19]. In condensed matter physics, this trick has been used for the first time in Ref. [20].

Within this method one replaces solving an equation

$$F(A) = 0, \tag{15}$$

where *F* is a matrix function of a matrix function *A*, and a subsequent calculation of a quantity  $B(A_0)$ , where  $A_0$  is the solution of Eq. (15), by an integral of the form

$$B = \int B(a)\delta(F(a)) \left| \det\left(\frac{\partial F}{\partial a}\right) \right| da.$$
(16)

The  $\delta$  function can be written as

$$\delta[F(a)] = C \int \exp[ifF(a)]df,$$

where *C* is a coefficient, and the determinant is obtained after integration of an exponential of a quadratic form in Grassmann variables  $\eta$  and  $\eta^+$ .

Our problem of solving Eq. (13) and calculation of the integral in Eq. (12) is of this type and we proceed following the above trick. We introduce anticommuting variables  $\theta$  and  $\theta^*$  and a superfield  $\Psi_{r,r'}(R)$ ,  $R = \{z, \theta, \theta^*\}$ ,

$$\Psi_{r,r'}(R) = a_{r,r'}(z)\theta + f_{r,r'}^T(z)\theta^* + \eta_{r,r'}(z) + \eta_{r,r'}^+(z)\theta^*\theta$$

where *a*, *f* are real and  $\eta$  is an anticommuting field. The field  $\Psi$  is periodic as a function of  $\tau$ ,  $\Psi(\tau) = \Psi(\tau + \beta)$ , but is anticommuting. The Hermitian conjugation "+" implies both the complex conjugation and transposition "*T*" with respect to *r*, *r*<sup>*l*</sup>.

As a result, one comes to an effective action quadratic in  $\Psi$  and linear in  $\phi_r(\tau)$ . This allows us to integrate over  $\phi_r(\tau)$  with the Gaussian weight of Eq. (7) and we come to the final expression for the partition function *Z*,

$$Z = Z_0 \int \exp(-S_0[\Psi] - S_B[\Psi] - S_I[\Psi]) D\Psi, \quad (17)$$

where  $S_0[\Psi]$  is the bare part of the action,

$$S_0 = \frac{i}{2} \sum_{r,r'} \int \left[ \Psi_{r',r} \left( \frac{\partial}{\partial \tau} + (\hat{\varepsilon}_r - \hat{\varepsilon}_{r'}) \right) \Psi_{r,r'} \right] dR,$$

and the interaction terms are given by

$$S_{B} = -\frac{V_{0}}{2} \sum_{r} \int \delta(\tau - \tau_{1}) \Psi_{r,r}(R) \\ \times \theta^{*} [\Psi_{r,r}(R_{1})\theta_{1}^{*} + 2i\Pi_{r}(R_{1})]\sigma\sigma_{1}dRdR_{1}, \\ S_{I} = \frac{V_{0}}{2} \sum_{r} \int \delta(\tau - \tau_{1})\Pi_{r}(R)\Pi_{r}(R_{1})\sigma\sigma_{1}dRdR_{1}, \\ \Pi_{r}(R) = u \sum_{r'} [(\Psi_{r',r}(R) - n_{r',r}\theta)(\Psi_{r,r'}(R) - n_{r,r'}\theta)].$$

Integration over *R* in Eq. (17) implies summation over  $\sigma$  and integration over u,  $\tau$ ,  $\theta$ ,  $\theta^*$ . The bare action  $S_0$  and the interaction term  $S_I$  are invariant under the transformation of the fields  $\Psi$ 

$$\Psi_{r,r'}(\theta,\theta^*) \to \Psi_{r,r'}(\theta+\kappa,\theta^*+\kappa^*) - \kappa n_{r,r'} \qquad (18)$$

with  $\kappa$  and  $\kappa^*$  being anticommuting variables, whereas the term  $S_B$  breaks the invariance. The invariance under the transformation (18) is stronger than the standard BRST symmetry for stochastic field equations (invariance under the transformation  $\Psi(\theta^*) \rightarrow \Psi(\theta^* + \kappa^*)$ ), Ref. [18], and reflects additional symmetries of Eq. (13). It differs from the full supersymmetry by the presence of the term  $\kappa n_{r,r'}$  in Eq. (18) but still can lead to interesting Ward identities.

The model described by Eq. (17) can be studied using standard methods of field theory. One can, e.g., expand in the interaction  $V_0$  or develop a renormalization group scheme analogous to that of Ref. [14]. In both cases, one can use the Wick theorem with rather simple contraction rules that follow from the form of the bare action  $S_0$ . We leave such calculations for future publications.

Neglecting the terms of third and fourth order in  $\Psi$  of  $S_B$  and  $S_I$ , the integral for partition function Z, Eq. (17), becomes Gaussian and yields an RPA-like expression,

$$Z \simeq Z_0 \exp\left[-\frac{T}{2} \sum_{\omega} \int \frac{d^d \mathbf{k}}{(2\pi)^d} \ln K\right],$$

$$K = 1 + V_0 \int \frac{n(\mathbf{p} - \mathbf{k}/2) - n(\mathbf{p} + \mathbf{k}/2)}{i\omega + \varepsilon(\mathbf{p} - \mathbf{k}/2) - \varepsilon(\mathbf{p} + \mathbf{k}/2)} \frac{d^d \mathbf{p}}{(2\pi)^d}.$$
(19)

The same result can be obtained using Eqs. (12) and (13) and neglecting the field  $\tilde{\phi}_r(\tau)$  in the left-hand side of Eq. (13).

In Eq. (19), (K - 1) is the contribution of noninteracting bosonic excitations. Considering their interaction originating from the cubic and quartic in  $\Psi$  term in Eqs. (17) one can fully describe the initial fermionic system. So, going beyond RPA, Eq. (19), is straightforward and this is a very important advantage with respect to the older bosonization schemes [10–13]. We are confident that the present scheme can improve the analysis of Ref. [14] of nonanalytical corrections to the Landau Fermi liquid theory and expect its usefulness for study of a large variety of problems of strongly correlated systems.

Now we sketch a possible route for MC simulations. Standard MC algorithms are based on using Eq. (8). However, for some important configurations of  $\phi_r(\tau)$  the fermionic determinant  $Z_f[\phi(\tau)]$  is negative, which makes the MC procedure inefficient. This is the famous sign problem.

Here we suggest to use instead of  $Z_f[\phi(\tau)]$  the functional  $Z_b[\phi(\tau)]$ , Eq. (12), that can be found solving Eq. (13). The solution of Eq. (13) and the function  $Z_b[\phi(\tau)]$  can be approximated using a Green function  $\mathcal{G}_{r,r';r_1,r'_1}^{\sigma,u\phi}(\tau,\tau_1)$  introduced as the solution of the equation

$$\left(\frac{\partial}{\partial \tau} + \mathcal{H}_{r,r'}(\tau)\right) \mathcal{G}_{r,r';r_1,r_1'}^{\sigma,u\phi}(\tau,\tau_1) = \delta(\tau-\tau_1)\delta_{r,r_1}\delta_{r',r_1'}$$

Then, we write the functional  $Z_b[\phi(\tau)]$  as

$$Z_{b}[\phi(\tau)] = Z_{0} \exp\left[-\sum_{\sigma,r,r_{1},r_{1}'} \sum_{i,j} \int_{0}^{1} \mathcal{G}_{r,r;r_{1},r_{1}'}^{\sigma,u\phi}(\tau_{i},\tau_{j}) \times \tilde{\phi}_{r}(\tau_{i})n_{r_{1},r_{1}'}\tilde{\Phi}_{r_{1},r_{1}'}(\tau_{j})\Delta^{2}du\right].$$
 (20)

Similarly to Eq. (8), we write the function  $G_{r,r;r_1,r'_1}^{\sigma,u\phi}(\tau_i, \tau_j)$  for  $\beta > \tau_i > \tau_j > 0$  in the form

$$G_{r,r';r_1,r_1'}^{\sigma,u\phi}(\tau_i,\tau_j) = \hat{P}_{r,r'}(\tau_i,\tau_j) \\ \times [1 - \hat{P}_{r,r'}(\tau_j,0)\hat{P}_{r,r'}(\beta,\tau_j)]^{-1} \delta_{r,r_1} \delta_{r',r_1'}.$$
(21)

Herein, the operator  $\hat{P}$  is given by the expression

$$\hat{P}_{r,r'}(\tau_i,\tau_j) = \prod_{i \ge l \ge j} \exp(-\mathcal{H}_{r,r'}(\tau_l,\sigma,u)\Delta) \qquad (22)$$

where the multipliers in the product are ordered in time growing from the right to the left. (Of course, one should discretize also the variable *u*.) The function  $G_{r,r';r_1,r_1'}^{\sigma,u\phi}(\tau_i, \tau_j)$ satisfies the symmetry relation

$$\mathcal{G}_{r,r';r_1,r_1'}^{\sigma,u\phi}(\tau_i,\tau_j) = -\mathcal{G}_{r_1',r_1;r',r}^{\sigma,u\phi}(\tau_j,\tau_i), \qquad (23)$$

which allows one to consider times  $\beta > \tau_i > \tau_i > 0$ .

The form of the Green function Eq. (21) is typical for bosons. By construction [see Eqs. (13) and (21)] it is real unless a singularity is present, in which case an imaginary part might be generated. We argue that a possible zero in the Bose denominator in Eq. (21) is compensated by the function  $\Phi_{r_1,r'_1}$ , Eq. (13), vanishing at  $r_1 = r'_1$ . Alternatively, one can antisymmetrize in the beginning the function G in  $r_1$ ,  $r'_1$  by antisymmetrizing the  $\delta$  functions in Eq. (13). This compensation is clearly seen in the RPA, Eq. (19).

In the absence of any singularity, the result is insensitive to the way of subdividing the interval  $(0, \beta)$  into slices and  $Z_b[\phi(\tau)]$  remains positive in the process of the calculation for any  $\phi_r(\tau_i)$  excluding the sign problem. Since Z can now be expanded in a sum of positive terms, we believe that this MC procedure can be efficient. The above derivation can be done using the "Ising spin" auxiliary field of Refs. [4,6] as well, which is usually preferable for MC computations.

In conclusion, the exact bosonization method presented here opens new possibilities of both numerical and analytical study of models of interacting fermions. There is a reasonable chance that this new formalism is free from the sign problem supposed to be generically NP-hard [7] or problems of equivalent complexity.

We thank Transregio 12 of DFG, and the French ANR for financial support. We are grateful to F. David, A. Ferraz, and O. Parcollet for very useful discussions.

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