Exact bosonization for an interacting Fermi gas in arbitrary dimensions

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(Dated: July 19, 2009)

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. We show schematically how the mapping can be used for Monte Carlo calculations and argue that it should be free from the sign problem. Introducing superfields we derive a field theory that may serve as a new way of analytical study.

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 re-summation 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 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 the model 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]. However, these schemes are applicable only for a long range interaction.

A more general low energy bosonization scheme suggested recently [13] is based on quasiclassical equations and can be used for an arbitrary range of the interaction. New logarithmic contributions to anomalous dependence of the specific heat [13] and spin susceptibility [14] were found. However, working well for $d = 1$ the scheme of Ref. [13] is not completely accurate for $d > 1$ because it does not fully accounts for all effects of the Fermi surface curvature [15].

All the previous bosonization methods are not exact; hence they cannot be used for accurate numerical studies of the initial fermionic problem.

In this paper, we present a new scheme that allows one to map models of 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 non-interacting bosons in an effective Hubbard-Stratonovich field with a subsequent integration over these fields or in a form of a supersymmetric field theory of superfields with quartic and cubic interactions. The former version may be convenient for MC study, while the latter one promises to be good for analytical investigations.

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

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

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

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

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

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

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 tunnelling from the site r to the site r', $V_{r,r'}$ is the electron-electron interaction between the r and r' and μ 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

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

which corresponds to an onsite repulsion.

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

$$\hat{H}_{int}^{(0)} = -\frac{V_0}{2}\sum_r \left(c_{r,+}^{+}c_{r,+} - c_{r,-}^{+}c_{r,-}\right)^2 \tag{5}$$

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

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

$$Z = Tr\exp\left(-\hat{H}/T\right). \tag{6}$$

Following a standard route of the Hubbard-Stratonovich transformation we decouple the interaction term, Eq. (5), integrating over an auxiliary real field $\phi(r,\tau)$, where τ is an imaginary time varying in the interval $0 \leq \tau < \beta$, $\beta = 1/T$. The field $\phi(r,\tau)$ is periodic in τ, such that $\phi(r,\tau) = \phi(r,\tau+\beta)$.

Proceeding in this way one obtains a model of non-interacting electrons in the external field $\phi(r,\tau)$. This allows one to calculate the trace over the electronic states and reduce the partition function Z to the form

$$Z = \int Z[\phi]\exp\left[-\frac{1}{2V_0}\sum_r\int_0^\beta \phi^2(r,\tau)\,d\tau\right]D\phi, \tag{7}$$

$$\begin{aligned} Z[\phi] &= \exp\left[\int_0^\beta Tr_{r,\sigma}\ln\left(-\partial/\partial\tau - \hat{h}_{r,\sigma} + \mu'\right)d\tau\right], \\ \hat{h}_{r,\sigma}(\tau) &= \hat{\varepsilon}_r - \sigma\phi_r(\tau)\ , \end{aligned} \tag{8}$$

where $\hat{\varepsilon}_r f_r \equiv -\sum_{r'} t_{r,r'} f_{r'}$ for an arbitrary function f_r and $Tr_{r,\sigma}$ means summation over r and σ.

In order to reduce the fermionic model, Eqs. (7-8), to a bosonic one, we first introduce an additional variable $0 \leq u \leq 1$ and write the function $Z[\phi]$ as [13]

$$Z[\phi] = Z_0\exp\left[\sum_{r,\sigma}\int_0^\beta\int_0^1 \sigma\phi_r(\tau)\,G_{r,r;\sigma}^{(u\phi)}(\tau,\tau+0)\,d\tau du\right] \tag{9}$$

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 satisfying

$$\begin{aligned} \left(-\frac{\partial}{\partial\tau} - \hat{h}_{r,\sigma}(u) + \mu'\right)G_{r,r';\sigma}^{(u\phi)}(\tau,\tau') &= \delta_{r,r'}\delta(\tau-\tau'), \\ \hat{h}_{r,\sigma}(\tau,u) = \hat{\varepsilon}_r - \sigma u\phi_r(\tau), \end{aligned} \tag{10}$$

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 look for the solution of Eq. (10) writing the Green function $G_{r,r';\sigma}^{(u\phi)}(\tau,\tau')$ as

$$G_{r,r';\sigma}^{(u\phi)}(\tau,\tau') = \sum_{r_1,r_2} T_{r,r_1;\sigma,u}(\tau)\,G_{r_1,r_2}^{(0)}(\tau-\tau')\,T_{r_2,r';\sigma,u}^{-1}(\tau')$$

where $G_{r_1,r_2}^{(0)}(\tau-\tau')$ is the Green function of the ideal Fermi gas and $T_{r,r';\sigma,u}(\tau)$ is an unknown function with the bosonic boundary condition $T_{r,r';\sigma,u}(\tau) = T_{r,r';\sigma,u}(\tau+\beta)$ and $T_{r,r';\sigma,u}^{-1}(\tau)$ is the inverse function,

$$\sum_{r''} T_{r,r''}(z)\,T_{r'',r'}^{-1}(z) = \delta_{rr'}, \quad z = (\tau,\sigma,u).$$

Substituting $G_{r;r';\sigma}^{(u\phi)}(\tau,\tau')$ into Eq. (10), we obtain equations for the functions $T_{r,r';\sigma,u}(\tau)$ and $T_{r,r';\sigma,u}^{-1}(\tau)$,

$$\begin{aligned} -\frac{\partial}{\partial\tau}T_{r,r'}(z) - (\hat{\varepsilon}_r - \hat{\varepsilon}_{r'})\,T_{r,r'}(z) + \sigma u\phi_r(\tau)\,T_{r,r'}(z) = 0, \\ \frac{\partial}{\partial\tau}T_{r,r'}^{-1}(z) + (\hat{\varepsilon}_r - \hat{\varepsilon}_{r'})\,T_{r,r'}^{-1}(z) + \sigma u\phi_{r'}(\tau)\,T_{r,r'}^{-1}(z) = 0. \end{aligned} \tag{11}$$

We can consider $T_{r,r'}(z)$ as a matrix with indices r, r', such that the sums of the space variables are simply matrix products. In principle, one could try to solve Eqs. (11) for the bosonic variable $T(z)$ and directly calculate the function $Z[\phi]$ but it is more convenient to introduce a new function $A_{r,r'}(z)$ as

$$A(z) = -[T(z),\hat{n}]\,T^{-1}(z), \tag{12}$$

where $[..,..]$ is the commutator and $\hat{n}$ is a matrix with the matrix elements $n_{r,r'}$ determined by the Fourier transform in $r-r'$ of the Fermi distribution

$$n(\mathbf{p}) = \left[\exp\left[\beta\left(\varepsilon(\mathbf{p}) - \mu'\right)\right] + 1\right]^{-1} \tag{13}$$

with $\varepsilon(\mathbf{p})$ being the electron energy corresponding to $\hat{\varepsilon}_r$. The function $A(\tau)$ is periodic, $A(\tau) = A(\tau+\beta)$.

The function $n_{r,r'}$ is just the Green function $G_{r,r'}^{(0)}(-0)$ and we can write the partition function $Z[\phi]$ in terms of the function $A(z)$ as

$$Z[\phi] = Z_0\exp\left[-\sum_{r,\sigma}\int_0^1\int_0^\beta \sigma\phi_r(\tau)\,A_{rr}(z)\,du d\tau\right]. \tag{14}$$

Remarkably, one can derive a closed equation for $A(z)$.

Let us consider $[...,\hat{n}]$ as an operator acting on any function f as $[...,\hat{n}]\,f = [f,\hat{n}]$. The equation for $A(z)$ can be obtained acting by the operator $[...,\hat{n}]$ on the first equation (11) for T and multiplying the obtained equation by T^{-1} from the right. Then, one has to multiply the second equation (11) for T^{-1} by $[T,\hat{n}]$ from the left and subtract the two obtained equations from each other. This gives the following equation for $A(z)$**:**

$$\begin{aligned} \frac{\partial}{\partial\tau}A_{r,r'}(z) &+ \mathcal{H}_{r,r'}(z)\,A_{r,r'}(z) = u\sigma\Phi_{r,r'}(\tau)\,n_{r,r'}, \\ \mathcal{H}_{r,r'}(z) &= \hat{h}_{r,\sigma}(\tau,u) - \hat{h}_{r',\sigma}(\tau,u) \end{aligned} \tag{15}$$

with $\hat{h}_{r,\sigma}(\tau,u)$ from Eq. (10) and

$$\Phi_{r,r'}(\tau) = \phi_r(\tau) - \phi_{r'}(\tau).$$

So, instead of calculating the fermionic determinant in Eq. (8) we are to solve the linear equation (15) for $A_{r,r'}(z)$ and substitute the solution into Eq. (14). This reduction is similar to the one of Ref. [13] developed in the quasiclassical approximation, whereas here all the transformations are exact. The partial differential equation (15) admits the parasitic solution $A_{r,r'}(z) = -un_{r,r'}$ which is not present in Eq. (10). It is excluded by complementing Eq. (15) with the constraint $Tr_r A = 0$ that follows from the definition of A, Eq. (12).

Eqs. (7, 14, 15) can serve as the starting point of both numerical and analytical investigations. For analytical studies it is convenient to represent the solution of Eq. (15) in a form of an integral over superfields, which allows to integrate over the field $\phi_r(\tau)$ in the beginning, thus reducing the model to a model of interacting bosons.

Let us start with the form suitable for analytical studies. We are to integrate over the field $\phi_r(\tau)$ exactly in order to derive a field theory for interacting bosons. In Ref. [13] 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 [16] (see also the book [17]). A similar transformation was used in the quantization of non-abelian gauge theories [18]. In condensed matter physics this trick has been used first in Ref. [19] in the context of stochastic equations.

Within this method one replaces solving an equation

$$F(A) = 0, \tag{16}$$

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. (16), by an integral of the form

$$B = \int B(a)\delta(F(a)) \left|\det\left(\frac{\partial F}{\partial a}\right)\right| da. \tag{17}$$

The δ-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 η and ρ.

Our problem of solving Eq. (15) and calculation of the integral in Eq. (14) is exactly of this type and we proceed following the above trick.

We introduce new anticommuting variables θ and θ^* and a superfield $\Psi_{r,r'}(R)$, $R = \{z, \theta, \theta^*\}$,

$$\Psi_{r,r'}(R) = a_{r,r'}(z)\,\theta + f^T_{r,r'}(z)\,\theta^* + \eta_{r,r'}(z) + \eta^+_{r,r'}(z)\,\theta^*\theta$$

where a, f are real and η is an anticommuting field. The field Ψ is periodic as a function of τ, $\Psi(\tau) = \Psi(\tau+\beta)$, but is anticommuting. The hermitian conjugation " $+$ " implies both the complex conjugation and transposition "T" with respect to r, r'.

As a result, one comes to an effective action quadratic in Ψ 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,

$$Z = Z_0 \int \exp\left[-S_0[\Psi] - S_B[\Psi] - S_I[\Psi]\right] D\Psi, \tag{18}$$

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

$$S_B = -\frac{V_0}{2}\sum_r \int \delta(\tau-\tau_1)\Psi_{r,r}(R)\,\theta^* \times\left[\Psi_{r,r}(R_1)\,\theta_1^* + 2i\Pi_r(R_1)\right]\sigma\sigma_1 dR dR_1\,,$$

$$S_I = \frac{V_0}{2}\sum_r \int \delta(\tau-\tau_1)\Pi_r(R)\,\Pi_r(R_1)\,\sigma\sigma_1 dR dR_1,$$

$$\Pi_r(R) = u\sum_{r'}\left[(\Psi_{r',r}(R) + n_{r,r'}\theta)(\Psi_{r,r'}(R) + n_{r,r'}\theta)\right]$$

Integration over R in Eq. (18) implies summation over σ 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 Ψ

$$\Psi_{r,r'}(\theta,\theta^*) \to \Psi_{r,r'}(\theta+\kappa, \theta^*+\kappa^*) + \kappa n_{r,r'} \tag{19}$$

with κ and κ^* being anticommuting variables, whereas the term S_B breaks the invariance. The invariance under the transformation (19) is stronger than the standard BRST symmetry for stochastic field equations (invariance under the transformation $\Psi(\theta^*) \to \Psi(\theta^*+\kappa^*)$), Ref. [17], and reflects additional symmetries of Eq. (15). It differs from the full supersymmetry by the presence of the term $\kappa n_{r,r'}$ in Eq. (19) but still can lead to interesting Ward identities.

The model described by Eqs. (18) 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 the one of Ref. [13]. In both the cases one can use the Wick theorem with simple contraction rules following from the form of the bare action S_0. We leave such calculations for future publications.

Neglecting cubic and quartic in Ψ terms in S_B and S_I in Eq. (18) one has a purely quadratic action and the partition function Z yields an RPA-like expression,

$$Z \simeq Z_0 \exp\left[-\frac{T}{2}\sum_\omega \int \frac{d^d\mathbf{k}}{(2\pi)^d}\ln K\right], \tag{20}$$

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

The same result can be obtained using Eqs. (14, 15) and neglecting the field $\phi_r(\tau)$ in the L.H.S. of Eq. (15).

In Eq. (20), $(K-1)$ is the contribution of non-interacting bosonic excitations. Considering their interaction one can fully describe the initial fermionic system.

In the remaining of this paper, we sketch a possible route for MC simulations. The supersymmetric form (18) obtained after the averaging over $\phi_r(\tau)$ is not proper for the numerical study and we want to show how one may calculate $Z[\phi]$ in a way suitable for the MC method. Following Ref. [3] one subdivides the interval $[0,\beta]$ into many slices $[\tau_i, \tau_i+\Delta\tau]$, $i=1,2,...,N$, where $\Delta\tau=\beta/N$. Then, one calculates $Z[\phi]$ for different $\tilde{\phi}_r(\tau_i)$ defined on the times τ_i. An efficient algorithm demands the positivity of $Z[\tilde{\phi}]$, which is not the case when using Eq. (8) directly. This is the famous sign problem.

We start with Eqs. (14-15). The solution of Eq. (15) and the function $Z[\phi]$ can be written in terms of a Green function $\mathcal{G}^{\sigma,u\phi}_{r,r';r_1,r_1'}(\tau,\tau_1)$ introduced as the solution of

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

Then, we obtain for the function $Z[\phi]$

$$Z[\phi] = Z_0\exp\Big[-\sum_{\sigma,r,r_1,r_1'}\int_0^1\int_0^\beta\int_0^\beta \mathcal{G}^{\sigma,u\phi}_{r,r;r_1,r_1'}(\tau,\tau_1) \times\phi_r(\tau)\,n_{r_1,r_1'}\Phi_{r_1,r_1'}(\tau_1)\,d\tau d\tau_1 du\Big]. \quad (21)$$

In analogy with the representation for the fermionic Green functions suggested in Ref. [3], we represent the function $\mathcal{G}^{\sigma,u\phi}_{r,r;r_1,r_1'}(\tau,\tau_1)$ for $\beta>\tau>\tau_1>0$ in the form

$$\mathcal{G}^{\sigma,u\phi}_{r,r';r_1,r_1'}(\tau,\tau_1)=\hat{P}_{r,r'}(\tau,\tau_1) \times\left(1-\hat{P}_{r,r'}(\tau_1,0)\,\hat{P}_{r,r'}(\beta,\tau_1)\right)^{-1}\delta_{r,r_1}\delta_{r',r_1'}. \quad (22)$$

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

$$\hat{P}_{r,r'}(\tau,\tau_1)=T_\tau\exp\left(-\int_{\tau_1}^{\tau}\mathcal{H}_{r,r'}(\tau'',\sigma,u)\,d\tau''\right) \quad (23)$$

where T_τ is the time ordering operator. The function $\mathcal{G}^{\sigma,u\phi}_{r,r';r_1,r_1'}(\tau,\tau_1)$ satisfies the symmetry relation

$$\mathcal{G}^{\sigma,u\phi}_{r,r';r_1,r_1'}(\tau,\tau_1)=-\mathcal{G}^{\sigma,u\phi}_{r_1',r_1;r',r}(\tau_1,\tau), \quad (24)$$

which allows also to consider times $\beta>\tau_1>\tau>0$.

The form of the Green function Eq. (22) is typical for bosons. By construction, 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. (22) is compensated by the function $\Phi_{r_1,r_1'}$, Eq. (15), vanishing at $r_1=r_1'$. Alternatively, one can antisymmetrize in the beginning the function $\mathcal{G}$ in r_1, r_1' by antisymmetrizing the δ-functions in Eq. (15). This compensation is clearly seen in the RPA, Eq. (20).

In the absence of any singularity, the result is insensitive to the way of subdividing the interval $[0,\beta]$ into the slices determining the operator $\hat{P}_{r,r'}$. Therefore, $Z[\phi]$ remains positive in the process of the calculation for any ϕ excluding the sign problem. Since Z can be expanded in a sum of positive terms, we believe that a procedure similar to the one of Refs. [3, 4] can be efficient within our new bosonization scheme.

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

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

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