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Boundary Conditions for Renormalization-Group Equations in One-Dimensional Fermi Gas

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(Received 7 September 1977)

The energy gap in one-dimensional Fermi systems with weak attractive interaction is expressed in terms of the parameters of the Hamiltonian and the electron density. The models of Hubbard and phonon-mediated interactions are studied in detail. The result for the Hubbard model is compared with numerical calculations.

As is well known, the energy spectrum of Fermi systems with attractive interaction has a gap. The purpose of this work is to derive an expression for the magnitude of the gap in a weakly interacting one-dimensional system. We obtain results for two systems: the Hubbard model and electron-phonon system.

The Hubbard Hamiltonian,

$$H=-T\sum_{i\sigma}(a_{i\sigma}^{\dagger}a_{i+1\sigma}+a_{i\sigma}^{\dagger}a_{i-1\sigma})+U\sum_{i}a_{i\uparrow}^{\dagger}a_{i\uparrow}a_{i\downarrow}^{\dagger}a_{i\downarrow}, \tag{1}$$

describes electrons on a lattice with nearest-neighbor hopping and interacting only when they are in one cell.

In the weak-coupling limit $|U/T|\ll 1$, $U/T<0$, our result for the energy gap is

$$\Delta=8(2/\pi)^{1/2}T\sin^2(\pi\rho/2)\sqrt{g}\,e^{-1/g}, \tag{2}$$

where ρ is the average number of electrons per cell, the dimensionless coupling constant g is defined as

$$g=U/v\pi,$$

and the Fermi velocity $v=2T\sin(\pi\rho/2)$.

The dependence of Δ on the coupling constant g can be obtained from the renormalization-group (RG) equations.[1-3] However, for the determination of the density-dependent factor in (2) it is necessary to know the boundary conditions for the integration of the RG equations.

In the RG method one integrates over those degrees of freedom which are characterized by wave vectors separated from the Fermi points by distances larger than some value k. The wave vector k is arbitrary but it is assumed that $k\ll k_F$, the Fermi momentum, so that the electronic spectrum is well approximated by a linear function of momentum. As a result one obtains an effective Hamiltonian which has the form

$$H_{\rm eff}=\sum_{|p|<k}vp(b_p^{\dagger}b_p-c_p^{\dagger}c_p)+\frac{\pi v}{L}\sum_{\substack{k_1k_2k_3k_4\\|k_i|<k}}\delta(k_1+k_2-k_3-k_4)[g_1b_{k_1\sigma}^{\dagger}c_{k_2\sigma'}^{\dagger}b_{k_3\sigma'}c_{k_4\sigma}+g_2b_{k_1\sigma}^{\dagger}c_{k_2\sigma'}^{\dagger}c_{k_3\sigma'}b_{k_4\sigma}$$
$$+g_3(b_{k_1\sigma}^{\dagger}b_{k_2\sigma'}^{\dagger}c_{k_3\sigma'}c_{k_4\sigma}+c_{k_1\sigma}^{\dagger}c_{k_2\sigma'}^{\dagger}b_{k_3\sigma'}b_{k_4\sigma})]. \tag{3}$$

The effective coupling constants depend on k and g_1 obeys the following RG equation

$$k\,dg_1/dk=g_1^2+\tfrac{1}{2}g_1^3+f(g_1), \tag{4}$$

where the first two terms were calculated by perturbation theory[3] and the function $f(g_1)$ is an unknown remainder about which we only need to know that for small g_1 it is of order (g_1).[4] We assume that the function f depends only on g_1 alone. This is consistent with the theories based on the bosonization of fermions[4] in which the Hamiltonian splits into two commuting parts, one of which contains only g_1. Equation (4) is valid when the

following two conditions are satisfied: $k \ll k_F$ and $kv \gg \Delta$.

Perturbation theory allows the calculation of the effective coupling constants g_i for the values of k such that

$$g \ln(k_F/k) \ll 1. \tag{5}$$

To find the values of g_i in this region to second order we evaluate the diagrams in Fig. 1. For the Hubbard model, the diagram (f) is independent of energy and momentum and gives an unimportant shift of the chemical potential. The diagram (e) is equal to zero. The diagrams (b), (c), and (d) cancel. From diagram (a) we obtain

$$g_1(k) = g - g^2 L(k), \tag{6}$$

where

$$L(k) = -\ln k + \ln[2\sin(\pi\rho/2)]. \tag{7}$$

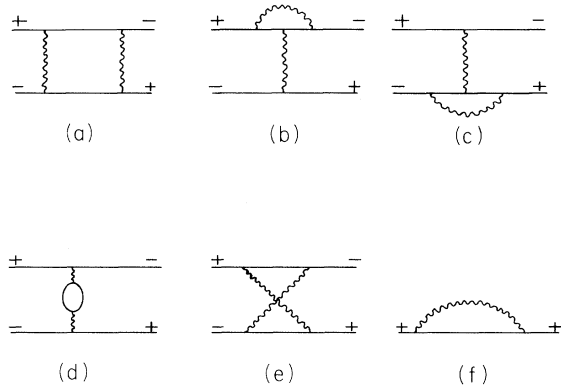

FIG. 1. Second-order diagrams for the vertex part and self-energy. The signs + and − on the lines stand for external momenta $+k_F$ and $-k_F$. External frequencies in the vertex part are zero relative to the Fermi level. In the self-energy graph the external frequency is $\omega \ll \omega_0$.

For small g, region of wave vectors satisfying (5) overlaps with the region in which (4) is valid. Therefore (6) can be used as a boundary condition for the RG equation (4). The integral of this equation is

$$L(k) = \frac{1}{g} - \frac{1}{g_1(k)} - \frac{1}{2}\ln\frac{g}{g_1(k)} - \int_g^{g_1(k)} d\bar{g}\left[\frac{1}{\bar{g}^2 + \frac{1}{2}\bar{g}^3 + f(\bar{g})} - \frac{1}{\bar{g}^2} + \frac{1}{2\bar{g}}\right]. \tag{8}$$

The integrand in the last term of (8) is nonsingular in the limit $g \to 0$, and to the required accuracy the lower bound can be replaced by zero.

In the region of small wave vectors k, where $g_1(k) \sim 1$, we cannot evaluate the integral in (8) since we do not know the function f in this region. However, the right-hand side of (8) is universal and does not depend on the details of the spectrum, in particular on the density of electrons.

We know from the work of Lieb and Wu[5] and Ovchinnikov[6] that the one-particle spectrum contains a gap Δ. For $k \lesssim \Delta/v$ Eq. (4) must be modified. We must add to its right-hand side a function $\varphi(\Delta/kv)$. Since the presence of Δ affects only an exponentially small region around the Fermi points, the function φ is independent of ρ. Thus for $vk \ll \Delta$ in the left-hand side of (8) $L(k)$ must be replaced by $L(\Delta/v)$ and on the right-hand side to one unknown constant we add another unknown constant. As a result (8) takes the form

$$L(\Delta/v) = C + g^{-1} - \tfrac{1}{2}\ln g, \tag{9}$$

where C is a numerical constant which cannot be determined by our methods. However, for $\rho = 1$ there exist an exact analytical solution[5,6]

$$\Delta = \frac{8T}{\pi g}\int_1^\infty dy \frac{(y^2-1)^{1/2}}{\sinh(y/g)} = \frac{8\sqrt{2}}{\sqrt{\pi}} T\sqrt{g}\, e^{-1/g}\left(1 + \frac{3g}{8} + \ldots\right). \tag{10}$$

Comparing (9) with (10) we obtain the value of C:

$$C = \ln(\pi^{1/2}/2^{3/2}). \tag{11}$$

Substituting this value of C into (9) we obtain the result (2). We note that in order to obtain the density dependence of the correction terms of relative order g we must evaluate the diagrams of perturbation theory in the third order.

It is interesting to compare formula (2) with the numerical calculation of Krivnov and Ovchinnikov[7] for the case of low densities, $\rho \ll 1$. They wrote the following expression for the gap:

$$\Delta = 2T\rho^2\pi(2/e)^{1/2}\exp(\pi^2\alpha_0)\sqrt{g}\,\exp(-1/g),$$

where α_0 was determined numerically: $\alpha_0 \simeq 0.11$. Formula (2) gives for α_0 the value

$$\alpha_0 = \frac{\ln\pi + 1}{2\pi^2} = 0.10865\ldots, \tag{12}$$

in good agreement with the numerical result.

Now we turn to the case of electron-phonon interaction. The RG equations (4) are the same[8] but the boundary conditions are specific for each model. In this case we have to evaluate the diagrams in Fig. 1 again, substituting for the wavy lines the phonon Green's functions multiplied by the square of the coupling constant. Since phonon frequencies are much smaller than electronic energies vk_F only phonons of wave vectors $2k_F$ and 0 are essential. Effective interaction mediated by these phonons is denoted by g and g_0, respectively. Evaluating the diagrams we find that the boundary condition has again the form (6) but the function $L(k)$ is replaced by a different function[9]

$$L_{ph}(k) = -\ln k + \ln[2tg(\pi\rho/2)] - 0.5. \quad (13)$$

Equation (9) is still valid with the substitution $L \rightarrow L_{ph}$. The energy gap is given as

$$\Delta_{ph} = 8(2/\pi e)^{1/2} T \frac{\sin^2(\pi\rho/2)}{\cos(\pi\rho/2)} \sqrt{g}\, e^{-1/g}. \quad (14)$$

This result is correct if the density ρ is not too close to 1: $T(1-\rho) \gg \omega_0$, where ω_0 is the frequency of phonons with momentum $2k_F$.

For nearly half-filled band, i.e., $T(1-\rho) \ll \omega_0$, it is necessary to include umklapp processes in diagrams (b) and (c). These contributions are equal to $\ln[2\pi T(1-\rho)/\omega_0]$. For $\rho \rightarrow 1$ this logarithmic singularity cancels the singularity in the second term of (13). For the gap in this case we get

$$\Delta_{ph}(\rho = 1) = 32(2/\pi e)^{1/2}(T^2/\omega_0)\sqrt{g}\, e^{-1/g}. \quad (15)$$

Equations (14) and (15) were derived under the assumption that the condition $g \ln k_F v/\omega_0 \ll 1$ is satisfied. This condition is, however, not essential. If it is not satisfied, in the expressions (14) and (15) for the gap it is only necessary to make the substitution in the factor $\sqrt{g} \rightarrow \sqrt{\tilde{g}}$, where $\tilde{g} = g/[1 - g\ln(k_F v/\omega_0)]$. It must still be $g \ll 1$ so that $\Delta \ll \omega_0$.

In (14) and (15) the preexponential factors are much larger, than ω_0. This is caused by the softening of $2k_F$ mode and the related enhancement of the electron-phonon coupling.

The method of this Letter is not limited to the concrete systems we studied. It can be applied to a wide class of model Hamiltonians with weak coupling. The parameters of the Hamiltonians must be determined either experimentally or by quantum-chemical calculations.

Work was supported in part by National Science Foundation Grant No. DMR76-23330A01 and by a grant from National Science Foundation in support of the Joint U.S.-U.S.S.R. Research Group.

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