Solution of the one-dimensional electron gas on a lattice

V. J. Emery*
Brookhaven National Laboratory, Upton, New York 11973

A. Luther† and I. Peschel†
Department of Physics, Harvard University, Cambridge, Massachusetts 02138
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An exact solution of the one-dimensional electron gas on a lattice is given for the special case in which two of the four coupling constants have particular values. It is shown that umklapp scattering has the same effect on the charge-density waves as backward scattering across the Fermi "surface" has on the spin-density waves and that the method of Luther and Emery can be used to solve this more general problem. For repulsive electron-electron interactions the umklapp scattering produces a gap in the charge-density wave spectrum and this appears for low-lying excitations when there is a half-filled band. The use of renormalization-group scaling to solve for general values of the coupling constants is discussed.

I. INTRODUCTION

In a recent solution[1] of the continuum one-dimensional electron gas, it was shown that, for attractive interactions, there is a gap in the spin-density wave spectrum, which has an important effect on the correlation functions at low temperatures[1,2] and introduces a new scale for their space and time variation. In particular, it was found that the uniform magnetic susceptibility is exponentially activated. The purpose of this paper is to point out that, if the background is not a continuum, but has a lattice periodicity, then, for repulsive electron-electron interactions, umklapp processes produce a gap in the charge-density wave spectrum which appears in the lowest excitations only when there is a half-filled band. In that case, it leads to an exponentially activated electrical conductivity.

In the continuum gas,[1] the charge-density waves are harmonic and they give power-law contributions to the correlation functions with exponents depending on the bare electron-electron coupling constants. On the other hand, the backward scattering which takes electrons from one Fermi point to another gives rise to an interaction between spin-density waves which is responsible for the existence of the energy gap.

With a lattice, the effects of umklapp scattering on the charge-density excitations are identical to those of backward scattering on the spin-density excitations.[1] The strategy for solving the problem is (i) to introduce a boson representation for the fermion operators which shows the separation into charge and spin-density excitations and the symmetry between them, (ii) to show that, for a particular value of two of the coupling constants, the charge- and spin-density Hamiltonians are separately equivalent to solvable fermion problems, and (iii) to solve for arbitrary values of the coupling constants by using the renormalization group to scale onto either the solvable value or to weak coupling.

The exact solution will be described in Sec. II and the use of renormalization-group scaling to solve the problem for coupling constants other than the special values will be discussed in Sec. III.

II. SOLUTION OF THE MODEL

The Hamiltonian for the system is

$$\mathcal{H} = \mathcal{H}_s + \mathcal{H}_L + \mathcal{H}_u, \tag{1}$$

where

$$\mathcal{H}_s = v_F \sum_{k,s} k(a^\dagger_{k,s} a_{k,s} - b^\dagger_{k,s} b_{k,s}) + 2L^{-1} \sum_k V \rho_1(k)\rho_2(-k), \tag{2}$$

$$\mathcal{H}_L = \sum_{s,s'} \int dx\, \psi^\dagger_{1,s}(x)\psi^\dagger_{2,s'}(x)\psi_{1,s'} \times (x)\psi_{2,s}(x)(U_\parallel \delta_{s,s'} + U_\perp \delta_{s,-s'}), \tag{3}$$

and the additional term which describes umklapp scattering is

$$\mathcal{H}_u = W_\perp \sum_s \int dx\, \psi^\dagger_{1,s}(x)\psi^\dagger_{1,-s}(x)\psi_{2,-s}(x)\psi_{2,s}(x)e^{-iGx} + \text{H.c.} \tag{4}$$

In these equations, the operators $a_{k,s}(b_{k,s})$ describe spin-$\frac{1}{2}$ fermions with momentum $k(-k)$, $\psi_{1,s}(x) = L^{-1/2}\sum_k e^{ikx} a_{k,s}$, $\psi_{2,s}(x) = L^{-1/2}\sum_k e^{ikx} b_{k,s}$ (where L is the length of the system); $\rho_1(k) = 2^{-1/2}\sum_{p,s} a_{p+k,s} a_{p,s}$ and $\rho_2(k) = 2^{-1/2}\sum_{p,s} b_{p+k,s} b_{ps}$ are

density operators and G is a reciprocal-lattice vector. We have implicitly assumed that the Fermi energy is sufficiently far from the band edge that linearization of the single-particle energy spectrum about the Fermi momentum is permissible.

We now introduce the boson representation for the fermion operators.[1,3,4] The Hamiltonian $\mathcal{H}_s$ and the $U_\parallel$ part of $\mathcal{H}_L$ constitute a Luttinger model and may be expressed in terms of the $\rho_j(k)$ and the spin-density operators $\sigma_1(k)=2^{-1/2}\sum_{p,s} s a^\dagger_{p+k,s}a_{ps}$ and $\sigma_2(k)=2^{-1/2}\sum_{p,s} s b^\dagger_{p+k,s}b_{p,s}$, all of which obey boson commutation relations.[3] For the umklapp term $\mathcal{H}_u$ and the backward scattering part of $\mathcal{H}_L$ (which is proportional to $U_\perp$) it is necessary to use the representation[4]

$$\psi_{j,s}(x)=(2\pi\alpha)^{-1/2}\exp\Big[\pm\Big(ik_F x+2\pi L^{-1}\sum_k k^{-1}\times\exp(-\tfrac{1}{2}\alpha|k|-ikx)\times 2^{-1/2}[\rho_j(k)+s\sigma_j(k)]\Big)\Big], \tag{5}$$

and the Hamiltonian then separates into a sum of a charge-density part $\mathcal{H}_\rho$ and a spin-density part $\mathcal{H}_\sigma$,

$$\mathcal{H}=\mathcal{H}_\rho+\mathcal{H}_\sigma, \tag{6}$$

with

$$\mathcal{H}_\rho=\frac{2\pi v_F}{L}\sum_k[\rho_1(k)\rho_1(-k)+\rho_2(-k)\rho_2(k)]+\frac{W_\parallel}{L}\sum_k\rho_1(k)\rho_2(-k)$$
$$+\frac{W_\perp}{(2\pi\alpha)^2}\int dx\exp\Big(\frac{2^{1/2}\pi}{L}\sum_k k^{-1}[\rho_1(k)+\rho_2(k)]\exp(-\tfrac{1}{2}\alpha|k|-ikx)+ix(G-4k_F)\Big)+\text{H.c.} \tag{7}$$

and

$$\mathcal{H}_\sigma=\frac{2\pi v_F}{L}\sum_k[\sigma_1(k)\sigma_1(-k)+\sigma_2(-k)\sigma_2(k)]-\frac{U_\parallel}{L}\sum_k\sigma_1(k)\sigma_2(k)$$
$$+\frac{U_\perp}{(2\pi\alpha)^2}\int dx\exp\Big(\frac{2^{1/2}\pi}{L}\sum_k k^{-1}[\sigma_1(k)+\sigma_2(k)]\exp(-\tfrac{1}{2}\alpha|k|-ikx)\Big)+\text{H.c.} \tag{8}$$

It can be seen that $\mathcal{H}_\sigma$ may be obtained from $\mathcal{H}_\rho$ by making the substitutions $\rho_j(k)\to\rho_j(k)$, $(W_\parallel, W_\perp)\to(-U_\parallel, U_\perp)$, and setting $G=4k_F$. The definition $W_\parallel=2V-U_\parallel$ has been used to make the notation symmetric. For $W_\perp=0$, $\mathcal{H}_\rho$ and $\mathcal{H}_\sigma$ are, respectively, $\mathcal{H}_0$ and $\mathcal{H}_1$ as defined in Eqs. (5) and (6) of Ref. 1. The Hamiltonian has then been separated into charge- and spin-density parts in Eq. (6) and they commute, since the $\rho_j(k)$ commute with the $\sigma_j(k)$. There is a similar separation of the correlation functions. The significance of the inclusion of umklapp processes is that the charge-density degrees of freedom have acquired an interaction which is just like the backward scattering term in the spin-density degrees of freedom. Now it has been shown[1] that for $U_\parallel(\pi V_F)^{-1}=-\frac{6}{5}$ there is a canonical transformation which reduces $\mathcal{H}_\sigma$ to the boson equivalent of a quadratic fermion Hamiltonian which is explicitly solvable and has an energy gap. Since the $\rho_j(k)$ and $\sigma_j(k)$ satisfy the same commutation relations, it is evident that there is a similar solution for $\mathcal{H}_\rho$ which may be obtained by replacing $\rho_j(k)$ for $\sigma_j(k)$ in the relevant steps of the original derivation.[1]

There are two differences. The first is that the solution occurs for $W_\parallel(\pi V_F)^{-1}=+\frac{6}{5}$, which is opposite to the sign required for $U_\parallel$. Of course, this is a consequence of the chosen sign convention, but it is appropriate because the Hubbard model[5] then corresponds to $U_\parallel=U_\perp=W_\parallel=W_\perp=U$. Thus the energy gap occurs in the spin-density spectrum for attractive forces and in the charge-density spectrum for repulsive interactions. The second difference is produced by the phase factor $e^{ix(G-4k_F)}$ which appears in Eq. (7). This has the consequence that the new fermion Hamiltonian representing the charge-density waves is

$$\mathcal{H}_{FC}=v_F'\sum_k k(c_k^\dagger c_k-d_k^\dagger d_k)+W_\perp(2\pi\alpha)^{-1}\times\sum_k(c_k^\dagger d_{k-2k_F'}+\text{H.c.}), \tag{9}$$

where $v_F'=\frac{4}{5}v_F$ and $2k_F'=G-2k_F$. This Hamiltonian has the eigenvalue spectrum $v_F'\{k_F'\pm[(k-k_F')^2+\Delta^{-2}]^{1/2}\}$ and $v_F'\{k_F'\pm[(k+k_F')^2+\Delta^{-2}]^{1/2}\}$ with $\Delta=W_\perp(2\pi\alpha)^{-1}$. Thus there are energy gaps at $k=\pm k_F'$. In the spin-density case, $k_F'=k_F$ always and the gap appears at the Fermi surface but, for the charge-density waves, this is true only for a half-

filled band, for which $G = 4k_F$. Only then, does the gap appear in the low-lying excitations. For other values of G, the solution might be compared to an intrinsic semiconductor.

As an example of the effects of the energy gap on the properties of the system, we calculate the zero frequency and wave-vector limit of the density correlation function whose behavior is analogous to that of the magnetic susceptibility for attractive interactions. Imagine that there is an external perturbation

$$\mathcal{H}' = \lambda \sum_{ks} (a_{ks}^\dagger a_{ks} + b_{ks}^\dagger b_{ks}) \tag{10}$$

applied to the system. This may be written in terms of the density operators $\rho_1(0)$ and $\rho_2(0)$ as above and then, after carrying out the transformations leading to Eq. (9), $\mathcal{H}'$ may be expressed as $\lambda \sum_k (c_k^\dagger c_k + d_k^\dagger d_k)$ which is a function of the new fermion variables. Then the required correlation function is

$$\chi_0 = \partial^2 E/\partial\lambda^2 = -2 \sum_k \partial f_k/\partial E_k, \tag{11}$$

where E_k are the eigenvalues of $\mathcal{H}_{FC}$ and f_k is the corresponding Fermi function. This is readily evaluated to give

$$\chi_0/L = \pi v_F' (2\pi\beta\bar{\Delta})^{1/2} e^{-\beta\bar{\Delta}} \tag{12}$$

at low temperatures.

A similar calculation shows that, in the presence of umklapp scattering the conductivity is exponentially activated.[6] This will be discussed in a separate publication.

III. RENORMALIZATION-GROUP SCALING

We shall now discuss the solution of the problem when $W_\parallel$ and $-U_\parallel$ are different from the solvable value $\frac{6}{5}\pi v_F$. This is likely to be necessary in practice since physically realized systems are expected to have the same sign for $W_\parallel$ and $U_\parallel$. For the more general case it is possible to use a renormalization-group-scaling argument as pointed out previously.[1] Since the spin- and charge-density degrees of freedom commute, scaling involves the $(U_\parallel, U_\perp)$ variables and the $(W_\parallel, W_\perp)$ variables separately, and, in each case, there are some regions in which the renormalization-group equations alone are sufficient to solve the problem and others where they may be used to scale onto our exact solution. We have derived third-order renormalization-group equations by calculating the effects of an infinitesimal variation of r — the range of the potential in momentum space — as in the method of Wegner and Houghton.[7] For the spin-density degrees of freedom, the changes in the coupling constants are given to third order by

$$\frac{d\bar{U}_\parallel}{dL} = -\bar{U}_\perp^2(1 + \tfrac{1}{2}\bar{U}_\parallel), \tag{13}$$

$$\frac{d\bar{U}_\perp}{dL} = -\bar{U}_\parallel\bar{U}_\perp - \tfrac{1}{4}(\bar{U}_\parallel^2 + \bar{U}_\perp^2)\bar{U}_\perp, \tag{14}$$

where $(\bar{U}_\parallel, \bar{U}_\perp)$ are the scaled values of $(U_\parallel/\pi V_F, U_\perp/\pi V_F)$ and $L = \ln(\bar{r}/r)$ ($\bar{r}$ is the new value of r). When $G = 4k_F$, the corresponding equations for the charge-density degrees of freedom are obtained by replacing $\bar{U}_\perp$ by $\bar{W}_\perp$ and $\bar{U}_\parallel$ by $-\bar{W}_\parallel$ in Eqs. (10) and (11). This is analogous to the scaling approach of Anderson, Yuval, and Hamann[8] for the Kondo problem but Eqs. (13) and (14) are taken to one higher order. Similar equations have been derived by Kimura,[9] who used different combinations of coupling constants. The advantage of the definitions used here is that the separation into charge- and spin-density wave parts is evident. To a great extent, Eqs. (13) and (14) may be guessed from the known isotropic form[10,11] $(U_\parallel = U_\perp)$ by using symmetry (invariance under reflection of $U_\perp$) and the fact that $U_\parallel$ is not renormalized when $U_\perp = 0$.

In order to discuss the solution of the problem for general values of $\bar{U}_\parallel$, L may be eliminated from Eqs. (13) and (14) and the resulting differential equation solved for $\bar{U}_\perp$ as a function of $\bar{U}_\parallel$ to give the scaling curves in the $(\bar{U}_\parallel, \bar{U}_\perp)$ plane:

$$(\bar{U}_\parallel^2 - \bar{U}_\perp^2)/(\bar{U}_\parallel + 2) = a, \tag{15}$$

where a is a constant. They are hyperbolas and relative to the solution[8] ($\bar{U}_\parallel^2 - \bar{U}_\perp^2 = \text{const}$) of the first-order scaling equations, they are displaced along the $\bar{U}_\parallel$ axis. Two properties of these equations determine the character of the solution. (i) From Eq. (15), the sign of $\bar{U}_\parallel^2 - \bar{U}_\perp^2$ is fixed, so the scaling curves do not cross the isotropic lines $\bar{U}_\parallel = \pm\bar{U}_\perp$. (ii) From Eq. (13), $d\bar{U}_\parallel/dL \leq 0$ for $\bar{U}_\parallel \geq -2$. Then, if $\bar{U}_\parallel \geq |\bar{U}_\perp|$, $\bar{U}_\perp$ must decrease and it becomes zero when $\bar{U}_\parallel^2 = (\bar{U}_\parallel + 4)a$. In this case the renormalization-group equations alone are sufficient to solve the problem and the second-order approximations (13) and (14) are adequate if the initial coupling constants are not too large. For the isotropic case, the result has been given by Menyhárd and Sólyom[11] and by Sólyom.[12] On the other hand, if $\bar{U}_\parallel < |\bar{U}_\perp|$, then $\bar{U}_\perp$ stays finite and both $\bar{U}_\parallel$ and $\bar{U}_\perp$ scale to the fixed point of Eqs. (13) and (14): $\bar{U}_\parallel = \bar{U}_\perp = -2$. Then Eqs. (13) and (14) are inadequate since their right-hand sides are expansions in powers of $\bar{U}_\parallel$ and $\bar{U}_\perp$, and the prediction of a fixed point at finite coupling cannot be trusted.

However the equations might be used as an approximate way of scaling onto $\bar{U}_{\parallel}=-\frac{6}{5}$, where our exact solution is valid.

This is an approximate procedure because the exact forms of the right-hand side of Eqs. (13) and (14) are unknown and also there are corrections to the equations themselves which become important as the coupling constant increases. Nevertheless, scaling with Eqs. (13) and (14) should be qualitatively correct provided there is no fixed point of the exact renormalization-group equations between the initial value of $\bar{U}_{\parallel}$ and $\bar{U}_{\parallel}=-\frac{6}{5}$. Finally there is another question that cannot be settled conclusively without a more detailed knowledge of the renormalization-group equations. When $\bar{U}_{\parallel}<|\bar{U}_{\perp}|$, Eqs. (13) and (14) allow scaling from $\bar{U}_{\parallel}>0$ to $\bar{U}_{\parallel}<0$, but it is not clear that this would be allowed by the exact renormalization-group equations. As we shall show, there is an exact homogeneity condition which suggests that the second-order expansion may be inadequate as $\bar{U}_{\parallel}\to 0$, with $\bar{U}_{\perp}$ finite. If so, we do not have even a qualitative solution for $0<\bar{U}_{\parallel}<|\bar{U}_{\perp}|$. All of the above remarks apply to the charge-density degrees of freedom for $G=4k_F$, if $(\bar{U}_{\parallel},\bar{U}_{\perp})$ are replaced by $(-\bar{W}_{\parallel},\bar{W}_{\perp})$.

With these provisos, it is possible to give a picture of the behavior of the system which is consistent with what is known for the Hubbard model[5] (corresponding to $U_{\parallel}=U_{\perp}=W_{\parallel}=W_{\perp}=U$). When $U_{\parallel}<0$ and $W_{\parallel}<0$, there is a gap in the spin-density wave spectrum and $W_{\parallel}$ scales to zero as $T\to 0$. The uniform magnetic susceptibility is exponentially activated. For $U_{\parallel}>0$ and $W_{\parallel}>0$, $U_{\parallel}$ scales to zero and the gap appears in the charge-density wave spectrum and it occurs for low-lying excitations only when there is a half-filled band. In this case the density response and electrical conductivity are exponentially activated.

For weak coupling, Eqs. (13) and (14) are sufficient to determine the analytic form of the energy gap, since the omitted higher-order terms give corrections which vanish as the coupling tends to zero. For isotropic coupling $\bar{U}_{\parallel}=\bar{U}_{\perp}=\bar{U}$, integration of the equations with the boundary condition that at $\bar{r}=r$, $\bar{U}=U_0/\pi v_F$ gives

$$\int_{U_0/\pi v_F}^{\bar{U}}\frac{dx}{x^2+\frac{1}{2}x^3}=-\ln(\bar{r}/r). \tag{16}$$

Here U_0 is the bare coupling constant. This equation shows that $\bar{U}$ is a function of $\bar{r}$ divided by a scale energy E_s which is

$$E_s=r^{-1}(|U_0|/\pi V_F)^{1/2}e^{\pi v_F/U_0} \tag{17}$$

for small U_0. The bare coupling constant enters only into E_s and this is the only thing which changes as U_0 varies. Thus, for weak coupling the energy gap is proportional to E_s and its analytic form given in Eq. (17) agrees with that obtained from the exact solution of the Hubbard model.[15]

IV. HOMOGENEITY OF THE PARTITION FUNCTION

In this section it will be shown that the partition function is homogeneous in T, L^{-1}, and powers of $U_{\perp}$ or $W_{\perp}$. This property gives direct information about the energy scale. The total partition function Z is a product of $Z_\sigma=\mathrm{Tr}\ e^{-\beta\mathcal{H}_\sigma}$ and $Z_\rho=\mathrm{Tr}\ e^{-\beta\mathcal{H}_\rho}$, and the derivation will be based upon an expansion of Z_σ in powers of $U_{\perp}$ and Z_ρ in powers of $W_{\perp}$. As pointed out by Luther and Emery,[1] this is analogous to the method used by Anderson, Yuval, and Hamann[8] for the Kondo problem, where the expansion was interpreted as the grand partition function for a classical gas. It is evident that a similar interpretation is possible here.[13]

It is simplest to use the boson form of $\mathcal{H}_\sigma$ given in Eq. (8). For the corresponding representation of the Kondo problem, the expansion has been discussed in great detail[14] and, following the same method, it is straightforward to show that

$$Z_\sigma=Z_0\sum_{m=0}^{\infty}\frac{\Delta^{2m}}{(m!)^2}\int_0^L\prod_i^{2m}dx_i \times\int_0^\beta\prod_j^{2m}dt_j\exp\Big(\sum_{p\neq q}^{2m}(-1)^{p-q}C_{pq}\Big), \tag{18}$$

where Z_0 is the partition function for $U_{\perp}=0$, $\Delta=U_{\perp}/2\pi\alpha$, and $C_{pq}=e^{-2\phi}\ln[(x_p-x_q)^2+v_F'^2(t_p-t_q)^2]/\alpha^2$. Here, as in Ref. 7, ϕ is given by $\tanh 2\phi=-U_{\parallel}/2\pi v_F$. If the time-ordering variables t_j are reinterpreted as space variables, the right-hand side of Eq. (18) is the grand partition function for a two-dimensional classical Coulomb gas.

Equation (18) may now be used to derive the homogeneity condition for the partition function in exactly the same way as in the Kondo problem.[15] Suppose β and L are divided by λ. Then, changing variables to $x_i'=\lambda x_i$ and $t_j'=\lambda t_j$ brings out a factor $\lambda^{-4m(1-e^{-2\phi})}$ in front of the integral in the term of order $2m$ and this may be removed by multiplying $U_{\perp}$ by $\lambda^{2(1-e^{-2\phi})}$. Since the x_i' and t_i' are dummy integration variables, the partition function is unchanged and it follows at once that Z_σ is a homogeneous function of degree zero in the variables T, L^{-1}, and $U_{\perp}^{1/2(1-e^{-2\phi})}$. This last quantity therefore gives the dependence of the energy scale upon $U_{\perp}$. For small $|U_{\parallel}|$, $e^{-2\phi}\approx 1+U_{\parallel}/2\pi v_F$ and the energy scale becomes $f(U_{\parallel})U_{\perp}^{-\pi v_F/U_{\parallel}}$. A similar result may be obtained for Z_ρ, replacing $(U_{\parallel},U_{\perp})$ by $(-W_{\parallel},W_{\perp})$.

If this is compared to the energy scale obtained from Eqs. (13) and (14) for arbitrary $U_{\parallel}$ and $U_{\perp}$, it is found that agreement is obtained only if $|U_{\perp}/U_{\parallel}| \ll 1$. [The result quoted in Eq. (17) is for $U_{\parallel} = U_{\perp}$.] A complete discussion of the circumstances in which one or other result is correct is not available at present, but the cutoff α appears to play a crucial role. Nevertheless, it is clear that, whenever the homogeneity condition gives the correct scale, it is not possible to use Eqs. (13) and (14) to allow $\bar{U}_{\parallel} \to 0$ with $\bar{U}_{\perp}$ finite.

V. OTHER MECHANISMS FOR ENERGY GAPS

It is important to realize that other mechanisms can also lead to a gap in the charge-density excitation spectrum and to essentially the same problem as discussed here. The two-strand model with inverted bands proposed[16] for tetrathiofulvolene tetracyanoquinodimethane leads to the same Hamiltonian as Eqs. (1)–(4) if we ignore spin and take $s = +1$ to refer to one strand and $s = -1$ to the other. In this situation, the half-filled-band criterion is always satisfied, and the gap is present for repulsive interactions between strands.[17] The electrical conductivity for these models is currently under investigation.

After this work had been completed we learned[18] that R. A. Klemm and H. Gutfreund had also noticed that the solution of the continuum electron gas[1] could be extended to deal with umklapp processes.

Note added in proof. Recently we were informed of similar results obtained by G. A. Kharadze at Tbilissi (U.S.S.R.) (private communication).

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