in agreement with the bulk interlayer spacing of 2.025 Å to within our estimated accuracy of ± 0.05 Å. In addition it compares with the conclusions of extensive multiple-scattering calculations.¹⁴

Further details of our method and applications to experimental data are given in forthcoming publications.^{4,8}

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¹C. J. Davisson and L. H. Germer, Phys. Rev. <u>30</u>, 705 (1927).

²Phys. Today <u>27</u>, No. 3, 17 (1974).

³U. Landman and D. L. Adams, J. Vac. Sci. Technol. 11, 195 (1974).

⁴D. L. Adams, U. Landman, and J. C. Hamilton, to

be published.

⁵M.J.Burger, *Vector Space* (Wiley, New York, 1954).

⁶J. C. Buchholz, M. G. Lagally, and M. B. Webb, Surface Sci. <u>41</u>, 248 (1974).

⁷T. A. Clarke, R. Mason, and M. Tescari, Surface

Sci. <u>30</u>, 553 (1972), and <u>40</u>, 1 (1973), and Proc. Roy. Soc., Ser. A <u>331</u>, 321 (1972).

⁸U. Landman and D. L. Adams, to be published.

⁹G. E. Laramore, Phys. Rev. B 6, 1097 (1972).

¹⁰L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1955).

¹¹R. V. Southwell, *Relaxation Methods in Theoretical*

Physics (Oxford Univ. Press, Oxford, England, 1946). ¹²C. B. Duke, N. O. Lipari, and U. Landman, Phys.

Rev. B <u>8</u>, 2454 (1973).

¹³The authors are indebted to Dr. J. E. Demuth and Dr. P. Marcus for supplying us with the phase shifts used in this calculation.

¹⁴D. W. Jepsen, P. M. Marcus, and F. Jona, Phys. Rev. B <u>5</u>, 3933 (1972).

Backward Scattering in the One-Dimensional Electron Gas*

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An exact solution to the one-dimensional electron gas with a particular attractive-interaction strength for scattering across the Fermi "surface" is given. It is shown that conductivity enhancement occurs for physically interesting values of the coupling constants. Scaling arguments are advanced to demonstrate that this solution applies generally for attractive backward scattering. In addition, the spinless problem is solved exactly for arbitrary couplings.

Progress towards an understanding of the equilibrium and transport properties of quasi-one-dimensional conductors has been hampered by a lack of knowledge about the underlying interacting electron system. Although the Tomonaga and Luttinger models¹ have provided some insight, their generality can be questioned as a result of their neglect of interactions near twice the Fermi momentum, $2k_{\rm F}$, which are responsible for backward scattering. This note reports an exact solution to the more general problem with an attractive interaction at $2k_{\rm F}$, and uses it to construct a qualitative picture for the general interacting one-dimensional system. Several properties of the exact solution are particularly significant. It requires an attractive interaction at $2k_F$ of a specific strength but the small-momentum interaction can be arbitrary, a situation of sufficient generality to be of interest for experiments on the quasi-one-dimensional systems. Depending upon the sign and magnitude of the small-momentum part, a large conductivity enhancement can occur as the temperature tends to zero, in contrast to a recent approximate treatment.² We compute the temperature dependence of the conductivity as well as other physically important response functions which describe the low-temperature pairing, charge and spin fluctuations, and magnetic susceptibility.

Together with the renormalization-group calculations of Menyhard and Sólyom,³ our solution can be used to provide a complete, if qualitative, picture of the one-dimensional interacting gas. This approach is analogous to the scaling argument of Anderson, Yuval, and Hamann for the Kondo problem.⁴

The model we solve is a logical extension of the Luttinger or Tomonaga model to include spin as well as interactions which scatter particles from $+k_{\rm F}$ to $-k_{\rm F}$. The Hamiltonian is the sum of free-particle kinetic energy, linearized near $k_{\rm F}$, plus the usual small-momentum interaction,⁵

$$\Im C_{s} = v_{F} \sum_{k,s} k (a_{k,s}^{\dagger} a_{k,s} - b_{k,s}^{\dagger} b_{k,s}) + 2L^{-1} \sum_{k} V \rho_{1}(k) \rho_{2}(-k),$$
(1)

where the operators $a_{k,s}$ $(b_{k,s})$ describe spin $-\frac{1}{2}$ fermions with momentum k $(-k)_{s}^{\circ} \rho_{1}(k)$ and $\rho_{2}(k)$ are density operators, $\rho_{1}(k) = 2^{-1/2} \sum_{j \in s} a_{j+k,s}^{\dagger} a_{j,s}$ and $\rho_{2}(k) = 2^{-1/2} \sum_{j \in s} b_{j+k,s}^{\dagger} b_{j,s}$. It is helpful in our subsequent discussion to introduce the spin-density operators $\sigma_{1}(k) = 2^{-1/2} \sum_{j \in s} a_{j+k,s}^{\dagger} a_{j,s}$ and $\sigma_{2}(k) = 2^{-1/2} \sum_{j \in s} s a_{j+k,s}^{\dagger} a_{j,s}$ and $\sigma_{2}(k) = 2^{-1/2} \sum_{j \in s} s a_{j+k,s}^{\dagger} a_{j,s}$ and $\sigma_{2}(k) = 2^{-1/2} \sum_{j \in s} s b_{j+k,s}^{\dagger} b_{j,s}$. With $s = \pm 1$. The operators ρ and σ satisfy the algebra of the Luttinger model, $[\rho_{1}(-k), \rho_{1}(+k')] = [\rho_{2}(+k), \rho_{2}(-k')] = \delta_{kk'} kL/2\pi$, together with identical equations for the σ commutators, $[\sigma_{1}(-k), \sigma_{1}(+k')] = [\sigma_{2}(+k), \sigma_{2}(-k')] = \delta_{kk'} kL/2\pi$, while all others vanish. The length of the sample is L and all states below $v_{F}k_{F}$ are filled. The kinetic energy term in Eq. (1) can be written in terms of these operators, by making use of well-known identities extended to the spin- $\frac{1}{2}$ case:

$$v_{\rm F} \sum_{k,s} k(a_{k,s}^{\dagger} a_{k,s} - b_{k,s}^{\dagger} b_{k,s}) - 2\pi v_{\rm F} L^{-1} \sum_{k} [\rho_1(k)\rho_1(-k) + \sigma_1(k)\sigma_1(-k) + \rho_2(-k)\rho_2(k) + \sigma_2(-k)\sigma_2(k)],$$

indicating a separation into density and spin-density operators.

The large-momentum-transfer terms are described by an additional \mathcal{R}_L in the form⁶

$$\mathcal{H}_{L} = \sum_{s,s'} \int dx \, \Psi_{1,s}^{\dagger}(x) \Psi_{2,s'}^{\dagger}(x) \Psi_{1,s'}(x) \Psi_{2,s}(x) [U_{\parallel} \delta_{s,s'} + U_{\perp} \delta_{s,-s'}], \tag{2}$$

where $\Psi_{1,s}(x) = L^{-1/2} \sum_{k} \exp(ikx) a_{k,s}$ and $\Psi_{2,s}(x) = L^{-1/2} \sum_{k} \exp(ikx) b_{k,s}$. The U_{\parallel} term can be written in terms of the density and spin-density operators by a permutation of the inner two operators, and becomes equal to

$$-U_{\parallel}L^{-1}\sum_{k}\rho_{1}(k)\rho_{2}(-k) - U_{\parallel}L^{-1}\sum_{k}\sigma_{1}(k)\sigma_{2}(-k).$$

The U_{\perp} term contains field operators of opposite spin, for which we use the boson representation^{7,8}:

$$\Psi_{j,s}(x) = (2\pi\alpha)^{-1/2} \exp\left\{\pm \left[ik_F x + 2\pi L^{-1} \sum_k k^{-1} \exp\left(-\frac{1}{2}\alpha |k| - ikx\right)\rho_{j,s}(k)\right]\right\},\tag{3}$$

where $v_F \alpha^{-1}$ is the bandwidth, $\rho_{1,s}(k) = \sum_{p} a_{p+k,s}^{\dagger} a_{p,s}$, $\rho_{2,s}(k) = \sum_{p} b_{p+k,s}^{\dagger} b_{p,s}$, and the plus (minus) sign goes with j = 1 (j = 2). This relationship has been discussed in detail for the spinless case⁷ and the generalization here is trivial, although the notation is somewhat cumbersome. This permits us to write the products of field operators in the U_{\perp} term as $(2\pi\alpha)^{-2} \exp\{2^{-1/2}[\varphi_1(x) + \varphi_2(x)]\}$, with

$$\varphi_{j}(x) = 2\pi L^{-1} \sum_{k} k^{-1} \exp\left(\frac{1}{2} \alpha |k| - ikx\right) \sigma_{j}(k).$$
(4)

The total Hamiltonian $\mathcal{K}_s + \mathcal{K}_L$ can now be written as the sum $\mathcal{K}_0 + \mathcal{K}_1$, where

$$\mathcal{H}_{0} = 2\pi v_{\rm F} L^{-1} \sum_{k} \left[\rho_{1}(k) \rho_{1}(-k) + \rho_{2}(-k) \rho_{2}(k) \right] + L^{-1} \sum_{k} (2V - U_{\parallel}) \rho_{1}(k) \rho_{2}(-k), \tag{5}$$

and

$$\mathcal{K}_{1} = 2\pi v_{\rm F} L^{-1} \sum_{k} [\sigma_{1}(k)\sigma_{1}(-k) + \sigma_{2}(-k)\sigma_{2}(k)] - L^{-1} \sum_{k} U_{\parallel}\sigma_{1}(k)\sigma_{2}(-k) + U_{\perp}(2\pi\alpha)^{-2} \int dx \left\{ \exp(2^{-1/2}[\varphi_{1}(x) + \varphi_{2}(x)]) + \text{H.c.} \right\},$$
(6)

and a separation into density and spin-density operators has been achieved. Obviously $[\mathcal{H}_1, \mathcal{H}_0] = 0$. It is interesting to note that the most general Hamiltonian for spinless fermions, $\sigma(k) = 0$, including large-momentum interactions is still of the Tomonaga-Luttinger form, for which the thermodynamics⁵ and correlation functions⁷ are known.

This separation into \Re_1 and \Re_0 is essential because \Re_0 is a quadratic form in boson operators and may be diagonalized by means of a canonical transformation. We now show that for a particular value

of U_{\parallel} , \mathcal{K}_{1} may also be diagonalized. Since the part of \mathcal{K}_{1} which does not involve U_{\perp} is quadratic it may be diagonalized by a transformation $e^{i\mathcal{S}}\mathcal{K}_{1}e^{-i\mathcal{S}}=\mathcal{K}_{1}'$, with $S=2\pi i L^{-1}\varphi\sigma_{1}(k)\sigma_{2}(-k)$, and $\tanh 2\varphi = -U_{\parallel} \times (2\pi v_{\rm F})^{-1}$. This transformation changes the velocity to $v_{\rm F}'=v_{\rm F}\operatorname{sech}2\varphi$ and the exponent of the U_{\perp} term to $2^{-1/2}e^{\varphi}[\varphi_{1}(x)+\varphi_{2}(x)]$. The point now is that if $2^{-1/2}e^{\varphi}=1$, comparison of Eqs. (3) and (6) shows that the U_{\perp} term is just the boson representation of a product of spinless Fermi fields $\Psi_{2}^{\dagger}(x)\Psi_{1}(x)\exp(-2i\times k_{\rm F}x)$. Writing the kinetic energy also in fermion representation, we find that \mathcal{K}_{1}' is quadratic and solvable:

$$\mathscr{K}_{1}' = v_{F}' \sum_{k} k (a_{k}^{\dagger} a_{k} - b_{k}^{\dagger} b_{k}) + U_{1} (2\pi\alpha)^{-1} \sum_{k} (a_{k}^{\dagger} b_{k+2k} + \text{H.c.}).$$

(7)

It is possible to make $2^{-1/2}e^{\varphi} = 1$ by choosing U_{\parallel} so that $\tanh 2\varphi = -U_{\parallel}(2\pi v_{\rm F})^{-1} = \frac{3}{5}$. Equation (7) has the eigenvalue spectrum $v_{\rm F}k_{\rm F} \pm [(k-k_{\rm F})^2 + \Delta^2]^{1/2}$ and $v_{\rm F}k_{\rm F} \pm [(k+k_{\rm F})^2 + \Delta^2]^{1/2}$, where $\Delta = U_{\perp} \times (2\pi\alpha)^{-1}$, indicating the appearance of gaps at $+k_{\rm F}$ and $-k_{\rm F}$. These gaps have important consequences for the properties of our solution.

The total Hamiltonian $\mathcal{K}' = e^{iS} \mathcal{K} e^{-iS} = \mathcal{K}_0 + \mathcal{K}_1'$ is now diagonalized, and it is straightforward to compute the free energy and correlation functions in the usual fashion. We may distinguish two regions: low temperatures, $T \ll \Delta$, for which the gap at the Fermi energy means that only excitations in \mathcal{K}_0 (and consequently density operators) are important; and high temperatures, $T \gg \Delta$, when the gap, and consequently U_{\perp} , are negligible. (A similar division applies to the frequency and momentum dependence.) In either case, the Hamiltonian is of the Tomonaga form, and the analytic behavior of correlation functions is therefore known from previous work.⁷

The properties of our solution are best expressed by the exponents characterizing the different spectral functions. These exponents are defined by $\text{Im}C(\omega) \propto \omega^{\mu}$, where C is the correlation function in question. Because the analytic form of these functions is of Tomonaga-Luttinger form, the temperature and momentum dependence is also determined by this exponent. The total scale dimension of these correlation functions is given by $\mu + 2$, the extra 2 resulting from two Fourier transforms in the definition of *C*. The exponents are listed in Table I, along with the temperature dependence of the magnetic susceptibility, for both low and high temperatures.

The electrical-conductivity relaxation rate in the impurity-dominated region is determined by the spectral function for the parallel-spin $2k_{\rm F}$ susceptibility,⁹ the characteristic energy W responsible for the interaction, and the free-particle conductivity σ_0 . The result in Table I then means that $\sigma = ne^2 \tau/m = \sigma_0 (T/W)^{-\mu}$, which will be enchanced ($\mu > 0$) whenever $v' < -\frac{2}{5}$. Under these conditions, the spectral density at $2k_{\rm F}$ vanishes, causing the reduction in scattering from the impurity.

It is interesting to compare with the renormalization-group approach of Menyhard and Sólyom.³ They considered the special case $U_{\parallel} = U_{\perp} = g_{\perp}$ and, for $g_1 < 0$, their exponents are qualitatively different from ours because they find that g_1 scales onto a fixed point $(g_1 = -2\pi v_F)$ which is outside the weak-coupling region for which their perturbation expansions are adequate. A more credible use of the renormalization-group equations, analogous to scaling theories of the Kondo problem,⁴ uses the fact that, provided no fixed point intervenes, the coupling constant would scale through the value $g_1 = -\frac{6}{5}\pi v_F$ at which our exact solution

TABLE I. Exponents of the spectral functions, defined in text, and the low- and high-temperature behavior of the magnetic susceptibility. The parameters $v' = V(\pi v_F)^{-1} + \frac{3}{5}$ and $\Delta = U_{\perp}(2\pi\alpha)^{-1}$.

Spectral function and operator	Low-temperature $(T \gg \Delta)$ exponent	$egin{array}{llllllllllllllllllllllllllllllllllll$
$\begin{array}{l} 2k_{\rm F} \text{ susceptibility, } \Psi_{1,+}^{\dagger}\Psi_{2,+}\\ 2k_{\rm F} \text{ susceptibility, } \Psi_{1,+}^{\dagger}\Psi_{2,-}\\ \text{Singlet pairing, } \Psi_{1,+}^{\dagger}\Psi_{2,-}^{\dagger}\\ \text{Triplet pairing, } \Psi_{1,+}^{\dagger}\Psi_{2,+}^{\dagger}\\ \text{Susceptibility, } \sigma_1 + \sigma_2 \end{array}$	$\begin{array}{c} -2 + [(1 - v')/(1 + v')]^{1/2} \\ -2 + [(1 - v')/(1 + v')]^{1/2} \\ -2 + [(1 + v')/(1 - v')]^{1/2} \\ -2 + [(1 + v')/(1 - v')]^{1/2} \\ (\pi v_{\rm F}')^{-1}(2\pi\beta\Delta)^{1/2} e^{-\beta\Delta} \end{array}$	$-\frac{3}{2} + [(1-v')/(1+v')]^{1/2} \\ [(1-v')/(1+v')]^{1/2} \\ -\frac{3}{2} + [(1+v')/(1-v')]^{1/2} \\ [(1+v')/(1-v')]^{1/2} \\ 2(\pi v_{\rm F})^{-1}(1-U_{\parallel}/2\pi v_{\rm F})^{-1}$

may be used. This suggests that the gap Δ exists for the weaker-coupling problems, $0 > g_1 > -\frac{6}{5}\pi v_F$, as well. If this gap exists, the low-temperature exponents given in Table I are still correct, with a new $v'2\pi v_F = 2V - U_{\parallel}$. The high-temperature exponents are more complicated but can be computed by setting $U_{\perp} = 0$, and following the usual procedure for the Tomonaga-model correlation functions.⁷

These exponents give substantial physical insight into the behavior of the system. For example, if the conductivity exponent is negative at high temperatures and positive at low temperatures a conductivity peak occurs at a temperature of the order of the gap, where the two power laws "cross over". The magnitude of this peak depends on W and U_{\perp} as well as the difference $\delta \mu$ between the two exponents. For $U_{\parallel}(\pi v_{\rm F})^{-1} = -\frac{6}{5}$, there can be a rather small peak because $\delta\mu$ is only $\frac{1}{2}$. We have calculated $\delta \mu$ for smaller $|U_{\parallel}|$, assuming that the scaling arguments are correct, and find that $\delta \mu$ approaches $\frac{6}{5}$ as $|U_{\parallel}| \rightarrow 0$. This is a new mechanism for a conductivity peak which merits a more detailed discussion than can be presented here.

Spin-flip impurity scattering will have a temperature dependence given by the opposite-spin $2k_{\rm F}$ susceptibility. Here the difference in exponents is large, indicating a stronger scattering at low temperatures which would dominate other mechanisms.

At the risk of making this problem appear more complicated (but even more intriguing), we now point out the reason behind our notation U_{\parallel} and U_{\perp} . These have been chosen to emphasize the connection to the Kondo parameters $-J_{\parallel}$ and J_{\perp} . The Hamiltonian in Eq. (6) has many similarities to the Tomonaga version of the Kondo Hamiltonian, and we expect many of the renormalizationgroup arguments to be applicable here as well. In particular, the weak-coupling scale energy for \Re_1 is $|U|^{1/2} \exp(-|U|^{-1})$, for $U_{\parallel} = U_{\perp} = U < 0$, as in the Kondo problem.

The inclusion of electron-phonon coupling

raises many questions for which there are only qualitative answers at present. In the adiabatic model, which views these interactions as giving rise to additional electron-electron coupling constants, the question of resistivity or conductivity enhancement depends sensitively on the relative signs and magnitudes of all coupling constants. Furthermore, if the phonon frequencies shift with temperature, these coupling constants also vary, and the calculation of the appropriate exponents becomes complicated. This problem is currently under investigation.

Much of this work was carried out while A. L. was a summer visitor at Brookhaven National Laboratory. The model solved in this paper appears to be related to generalizations of the Thirring model,¹⁰ as pointed out to us by S. Coleman.

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¹E. H. Lieb and D. C. Mattis, *Mathematical Physics* in One Dimension (Academic, New York, 1966).

²H. Fukuyama, M. Rice, and C. Varma, to be published.

³N. Menyhard and J. Sólyom, J. Low Temp. Phys. <u>12</u>, 529 (1973); J. Sólyom, J. Low Temp. Phys. <u>12</u>, 547 (1973).

⁴P. W. Anderson, G. Yuval, and D. R. Hamann, Phys. Rev. B <u>1</u>, 4464 (1970).

⁵D. C. Mattis and E. H. Lieb, J. Math. Phys. <u>6</u>, 304 (1965).

⁶There are many equivalent representations of these terms, and our notation is convenient for later purposes. The Hubbard model requires selecting $V = U_{\parallel} = U_{\perp}$, for which case the parallel-spin interactions cancel, while the notation of Ref. 3 corresponds to the choice $U_{\parallel} = U_{\perp} = g_1$ and $V = g_2$.

⁷A. Luther and I. Peschel, Phys. Rev. B <u>9</u>, 2911 (1974).

⁸D. Mattis, J. Math. Phys. <u>15</u>, 609 (1974).

⁹A. Luther and I. Peschel, Phys. Rev. Lett. <u>32</u>, 992 (1974).

 10 R. Dashen and Y. Frishman, Phys. Lett. <u>46B</u>, 439 (1973).