Momentum Distribution in the Tomonaga Model*

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The momentum distribution function for the ground state of the one-dimensional Tomonaga model at T=0 is derived. The applicability of the model is discussed. It is found that the restriction on the strength of the interaction is actually much weaker than that suggested by Tomonaga. The behavior of the distribution function near the Fermi momentum is investigated.

1. INTRODUCTION

NE of the pioneering steps in the theory of large systems of interacting fermions was made by Tomonaga,¹ who showed, using Bloch's method of sound waves,² that a one-dimensional assembly of electrons can be described in terms of collective degrees of freedom which behave approximately as bosons. Such collective modes are also manifested in threedimensional systems. In the case of the electron gas they are generally known as plasmons. However, the nature of the excitation spectrum in one and three dimensions is essentially different. The main difference lies in the fact that the excitation spectrum of the threedimensional system consists of single-particle excitations as well as of collective modes, while in Tomonaga's one-dimensional model there are only collective modes.³ Therefore the Tomonaga model can, and in fact does, lead to some results which are not valid in three dimensions. However, it provides an instructive and clear demonstration of the collective modes sustained in interacting-fermion systems.

The work of Little⁴ on superconductivity in long organic molecules has revived the interest in onedimensional models for practical reasons. Such molecules behave approximately like one-dimensional systems, and it seems that the Tomonaga model applies to this case. This model was used by one of us⁵ to investigate the possibility of flux quantization in a onedimensional ring.

The operators of the Tomonaga model which create eigenstates of the total Hamiltonian obey boson commutation relations only when evaluated within a subspace of functions, all of which have a filled core in k space, i.e., have no holes in a certain interval $[-k^*, k^*], k^* < k_F$, where k_F is the Fermi momentum.

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 ¹ S. Tomonaga, Progr. Theoret. Phys. (Kyoto) 5, 544 (1950).
 ² F. Bloch, Z. Physik 81, 363 (1933); Helv. Phys. Acta 7, 385 (1934).
 ³ This important fact was overlooked in the original paper of Tomonaga. It was pointed out by Overhauser [Physics 1, 307

Tomonaga. It was pointed out by Overhauser [Physics 1, 307 [1965] in the case of the Luttinger model. A rigorous proof was given by M. Schick (Ref. 5).
⁴ W. A. Little, Phys. Rev. 134, A1416 (1964).
⁵ M. Schick (to be published).

Tomonaga argues that for sufficiently weak long-range interactions and for sufficiently low temperatures, all the relevant states belong to this subspace. The main purpose of the present paper is to check this assumption a posteriori for the interacting ground state at T=0. To do this, we calculate the momentum distribution function in the ground state and thereby determine to what extent the states within the core $[-k^*, k^*]$ are actually filled. We employ the method used by Mattis and Lieb⁶ in their treatment of the Luttinger model.⁷ This is an exactly soluble one-dimensional model, similar to the Tomonaga model, but one which avoids the approximations inherent in the latter by an artificial distinction between particles of opposite momenta and the introduction of an infinite sea of negative energy particles.

The Tomonaga and Luttinger models are reviewed briefly in Sec. 2, and their relation is discussed.

In Sec. 3, the momentum distribution function in the interacting ground state is calculated. The results are similar to those obtained in the Luttinger model.⁶ The behavior of the momentum distribution at $k = k_F$ is also discussed.

2. TOMONAGA AND LUTTINGER MODELS

Consider a system of fermions on a line of length L. Assuming periodic boundary conditions, we may write the second quantized particle field in terms of plane waves as

$$\psi(x) = (1/\sqrt{L}) \sum_{n} c_n \exp(ik_n x),$$

$$k_n = (2\pi/L)n, \quad n = 0, \pm 1, \cdots, \quad (2.1)$$

where c_n and its Hermitian conjugate c_n^* are the fermion creation and destruction operators obeying the anticommutation relations

$$\{c_n, c_{n'}^*\} = \delta_{nn'}$$

The spin index will be omitted, as the spin plays no role in our discussion. Similarly, the particle density may be expanded as

$$\rho(x) = \psi^*(x)\psi(x) = (1/L)\sum_{n} \rho_n \exp(ik_n x), \quad (2.2)$$

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⁶ D. Mattis and E. Lieb, J. Math. Phys. **6**, 304 (1965). ⁷ J. M. Luttinger, J. Math. Phys. **4**, 1154 (1963).

where

$$\rho_n = \sum_l c_l^* c_{l+n}. \tag{2.3}$$

Following Tomonaga, we decompose the operators ρ_n into two parts:

$$\rho_n = \rho_n^{-+} + \rho_n^{-},$$

$$\rho_n^{+} = \sum_{l \ge -1/2n} c_l^* c_{l+n},$$

$$\rho_n^{-} = \sum_{l < -1/2n} c_l^* c_{l+n}.$$
(2.4)

The operators ρ_n^{\pm} in general satisfy complicated commutation relations, but Tomonaga showed that these simplify considerably if it is understood that the commutators are always to be evaluated acting on a subspace S of functions in the neighborhood of the noninteracting ground-state function. These functions are specified by the absence of holes in a certain interval $[-n^*, n^*], n^* < n_F, \text{ where } n_F = (L/2\pi)k_F.$ The lowenergy excited states of the noninteracting system are characterized by the existence of particles and holes near the Fermi level. The interaction causes virtual transitions of particles and thus mixes into the unperturbed states complicated configurations of particles and holes. Hopefully, if the force is not too strong and its range not too short, the new states will still belong to the subspace S. Within this subspace, the operators ρ_n^{\pm} satisfy, for $|n|, |n'| < \frac{2}{3}n^*$, the following bosonlike commutation relations¹:

$$[\rho_{n}^{+}, \rho_{n'}^{+}] = n\delta_{n,-n'}, [\rho_{n}^{-}, \rho_{n'}^{-}] = -n\delta_{n,-n'}, [\rho_{n}^{+}, \rho_{n'}^{-}] = 0.$$
 (2.5)

Since our treatment is restricted to states with particles and holes near the Fermi maximum, we can approximate the free-particle energy which is quadratic in the momentum by a linear expression

$$k^{2}/2m = (1/2m) (k_{F} + k - k_{F})^{2} \approx (1/2m) (-k_{F}^{2} + 2kk_{F}),$$
(2.6)

neglecting $(k-k_F)^2$. This results in the important feature of the Tomonaga model that the excitation energy of collective modes is proportional to the momentum. Tomonaga showed that the expression

$$H_{\text{K.E.}} = (2\pi\hbar/L)^2 (n_F/m) \sum_{n>0} (\rho_{-n}+\rho_n+\rho_n-\rho_{-n}) \quad (2.7)$$

is equivalent to within a constant to the Hamiltonian of the noninteracting system.⁸ This constant is equal to

the kinetic energy of the filled Fermi sea, so that $H_{\text{K},\text{E}}$. may be called the "excitation kinetic energy." The operators ρ_{-n}^+ , ρ_n^- and ρ_n^+ , ρ_{-n}^- are the raising and lowering operators of $H_{\text{K},\text{E}}$, respectively.

Any two-body interaction of the form

$$H_{I} = \frac{1}{2} \iint \rho(x) \rho(x') J(|x-x'|) dx dx' - \frac{1}{2} \int \rho(x) J(0) dx$$
(2.8)

can be expressed in terms of the density-fluctuation operators of Eq. (2.3) as

$$H_{I} = \frac{1}{2} \sum_{n \neq 0} \rho_{n} \rho_{-n} J_{n} + \frac{1}{2} \rho_{0}^{2} J_{0} - \frac{1}{2} \rho_{0} J(0), \qquad (2.9)$$

where

$$J_n = J_{-n} = (1/L) \int J(x) \, \exp(ik_n x) \, dx. \quad (2.10)$$

For the Tomonaga model to be applicable, it is necessary that the Fourier components of the interaction be negligible for $n > \frac{2}{3}n^*$, i.e., that the interaction be of sufficiently long range. Although all sums over n will effectively extend only up to a certain $n \le \frac{2}{3}n^*$, we shall formally write them as sums over all n.

The full Hamiltonian $H_{K,E}+H_I+$ const can be diagonalized by a canonical transformation generated by the operator

$$G = i \sum_{n}' (\theta_n/n) \rho_{-n}^+ \rho_n^-, \qquad (2.11)$$

where

$$\theta_n = \frac{1}{4} \ln(1 + N J_n / 2\epsilon_F). \qquad (2.12)$$

The prime on the sum denotes that the term with n=0 is excluded, and N is the total number of particles. Clearly, this transformation can only be valid provided that

$$J_n > -2\epsilon_F / N \tag{2.13}$$

for all n. Thus far there is only a restriction on the strength of attractive interactions, while repulsive interactions may be of any strength. In Sec. 3, we shall derive more stringent conditions on the strength of the interaction by requiring that the interacting ground state belongs to S. The raising and lowering operators of the interacting system are⁵

$$\widetilde{\rho}_{n}^{\pm} = e^{-iG} \rho_{n}^{\pm} e^{iG}$$
$$= \rho_{n}^{\pm} \cosh\theta_{n} - \rho_{n}^{\mp} \sinh\theta_{n}. \qquad (2.14)$$

The basic features of the Tomonaga model are the boson commutation relations (2.5) and the linear freeparticle spectrum. Both features are approximate. The Luttinger model^{6,7} shares these two features with the Tomonaga model. In this model, however, they are exact, since a linear spectrum is assumed from the beginning, and since boson characteristics of the corre-

⁸ It is shown in Ref. 5 that if one takes the true quadratic-energy spectrum, it is still possible to express the kinetic energy in terms of the ρ_n operators, but the expression also contains trilinear terms. It may be shown that under conditions which justify Eq. (2.6), the contribution of these terms is negligible, and one is left with Eq. (2.7).



FIG. 1. Comparison between the Luttinger and Tomonaga models. For explanation, see the text.

sponding operators are achieved by assuming two kinds of particles, one with the energy spectrum $\epsilon(k) = k$, and the other $\epsilon(k) = -k$. The particle field is

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = (1/\sqrt{L}) \sum_n \exp(ik_n x) \begin{pmatrix} c_{1n} \\ c_{2n} \end{pmatrix}, \quad (2.15)$$

where c_{1n} , c_{2n} are the destruction operators for the two kinds of particles, which satisfy the usual anticommutation relations

$$\{c_{sn}, c_{s'n'}^*\} = \delta_{ss'}, \delta_{nn'} \qquad (2.16)$$

and all the other anticommutators are zero. The Hamiltonian of the free system is

$$H_{0} = (v/\hbar) \int_{0}^{L} dx \psi^{*}(x) \sigma_{3} p \psi(x)$$

= $v \sum_{n} (c_{1n}^{*} c_{1n} - c_{2n}^{*} c_{2n}) k_{n},$ (2.17)

where p is the ordinary momentum operator, and σ_3 is the Pauli spin matrix. To ensure a finite ground-state energy, Luttinger postulates the existence of a filled sea of negative energy particles as in the Dirac theory of electrons. The two-body interaction is taken to be of the form

$$H_{\rm int} = \lambda \iint_{0}^{L} dx dx' \,\rho_1(x) \rho_2(x') J(|x-x'|). \quad (2.18)$$

Mattis and Lieb, in their treatment of the Luttinger model, defined certain operators which, in order to stress their similarity to the ρ_n operators of the Tomonaga model, we write as

$$\rho_{s,n} = \sum_{l} c_{s,l} * c_{s,l+n}, \quad s = 1, 2.$$
(2.19)

These operators satisfy the following commutation

relations:

$$[\rho_{1n}, \rho_{1n'}] = n\delta_{n,-n'},$$

$$[\rho_{2n}, \rho_{2n'}] = -n\delta_{n,-n'},$$

$$[\rho_{1n}, \rho_{2n'}] = 0.$$

$$(2.20)$$

The operators $\rho_{1,n}$, $\rho_{2,-n}$ and $\rho_{1,-n}$, $\rho_{2,n}$ are the raising and lowering operators for H_0 . The full Hamiltonian may be written as a bilinear form in these operators and diagonalized by a canonical transformation similar to Eq. (2.11), but with different θ_n .

The similarity between the two models can be visualized graphically. Figure 1(a) shows the singleparticle spectrum of the Luttinger model, with the two lines corresponding to the two kinds of particles. The Tomonaga model assumes holes and excited particles only near k_F and replaces sections of the parabola $\epsilon(k) = k^2/2m$ by straight lines. Since there are no holes and excited particles if |k| differs appreciably from k_F , the single-particle spectrum in those regions makes no difference, and we can continue the straight lines indefinitely, obtaining a spectrum identical to that of Fig. 1(a), provided that v is chosen to be the Fermi velocity $v_F = \hbar k_F/m$ [Fig. 1(b)].

3. MOMENTUM DISTRIBUTION

To calculate the momentum distribution in the Tomonaga model, we introduce a Fourier transform like that in Ref. 6, but instead of calculating $n(k_n)$ —the number of particles of momentum k_n —we prefer to start with the expression for the number of holes. The number of holes is given by

$$1 - n(k_n) = L^{-1} \iint_{-L/2}^{L/2} dx dx' \exp[ik_n(x - x')] I(x', x),$$
(3.1)

where

where

$$I(x', x) = \langle \tilde{0} \mid \psi(x')\psi^*(x) \mid \tilde{0} \rangle$$
$$= \langle 0 \mid e^{iG}\psi(x')\psi^*(x)e^{-iG} \mid 0 \rangle. \qquad (3.2)$$

Here $|\tilde{0}\rangle$ is the exact ground state, $|0\rangle$ is the noninteracting ground state, and G is given by Eq. (2.11). The particle field is separated into positive- and negative-momentum parts

$$\psi_{+}(x) = (1/\sqrt{L}) \sum_{n \ge 0} c_n \exp(ik_n x),$$

$$\psi_{-}(x) = (1/\sqrt{L}) \sum_{n < 0} c_n \exp(ik_n x), \qquad (3.3)$$

with similar expressions for $\psi_+^*(x)$ and $\psi_-^*(x)$. The function I(x', x) can be decomposed into four terms as follows:

$$I(x', x) = I_{++} + I_{+-} + I_{-+} + I_{--}, \qquad (3.4)$$

$$I_{\pm \pm} = \langle \tilde{0} | \psi_{\pm}(x')\psi_{\pm}^{*}(x) | \tilde{0} \rangle.$$
 (3.5)

The expressions I_{+-} and I_{-+} are easily seen to vanish.

For example,

$$I_{+-}(x', x) = (1/L) \sum_{n>0, m<0} \exp(ik_n x')$$
$$\times \exp(-ik_m x) \langle \tilde{0} \mid c_n c_m^* \mid \tilde{0} \rangle \quad (3.6)$$

vanishes, since all the matrix elements in the sum vanish because of momentum conservation. The remaining two terms are

$$I_{++} = (1/L) \sum_{n>0} \exp[ik_n(x'-x)] \langle \tilde{0} | c_n c_n^* | \tilde{0} \rangle,$$

$$I_{--} = (1/L) \sum_{n<0} \exp[ik_n(x'-x)] \langle \tilde{0} | c_n c_n^* | \tilde{0} \rangle. \quad (3.7)$$

Since we have not introduced any external potential to affect the symmetry of the momentum distribution, it follows that

$$\langle \tilde{0} \mid c_n c_n^* \mid \tilde{0} \rangle = \langle \tilde{0} \mid c_{-n} c_{-n}^* \mid \tilde{0} \rangle, \qquad (3.8)$$

from which we conclude that

$$I_{++}(x', x) = I_{--}(x, x').$$
 (3.9)

Let us now proceed to calculate I_{++} . We define a "state" vector $[f_{\sigma}(x))$:

$$|f_{\sigma}(x)\rangle = \exp(i\sigma G)\psi_{+}^{*}(x) \exp(-i\sigma G) |0\rangle,$$
 (3.10)

so that

$$I_{++}(x', x) = \langle f_{\sigma}(x') | f_{\sigma}(x) \rangle_{\sigma=1}.$$
(3.11)

Differentiating with respect to σ , we obtain

$$(\partial/\partial\sigma) | f_{\sigma}(x) \rangle = i \exp(i\sigma G) [G, \psi_{+}^{*}] \exp(-i\sigma G) | 0 \rangle.$$
(3.12)

To proceed, we need the following commutation relations:

$$[\rho_n^+, \psi_+^*] = \exp(-ik_n x)\psi_+^*(x) + \exp(-ik_n x)(1/\sqrt{L}) \sum_{-n/2 < l < 0} \exp(-ik_l x)c_l^*, \qquad n > 0$$

= $-\exp(-ik_n x)(1/\sqrt{L}) \sum_{0 < l < [n]} \exp(-ik_l x)c_l^*, \qquad n < 0$

$$[\rho_n^-, \psi_+^*(x)] = \exp(-ik_n x) (1/\sqrt{L}) \sum_{-n \le l < -n/2}^{-1} \exp(-ik_l x) c_l^*, \qquad n > 0$$

= 0 $n < 0. \quad (3.13)$

$$=0$$

These commutation relations are rather complicated, but they appear in Eq. (3.12) in the commutator $[G, \psi_{+}^{*}]$, which acts on the state $\exp(-i\sigma G) \mid 0$. For $\sigma = 1$, this is the exact ground state of the system, and we assume that it has no holes in the interval $[-n^*, n^*]$. The effect of multiplying G by a positive number σ is, according to Eq. (2.12), to replace J_n by a fictitious $J_n(\sigma)$ which is related to J_n by

$$(1+NJ_n/2\epsilon_F)^{\sigma}=1+NJ_n(\sigma)/2\epsilon_F.$$
 (3.14)

The fictitious interaction is weaker or stronger than the actual one for σ less or greater than one, respectively.

It is clear that if our assumption on the absence of holes in the core $[-n^*, n^*]$ holds for $\sigma = 1$, it certainly holds for $0 < \sigma < 1$, and we assume that it is also valid for values slightly greater than one. It is now straightforward to evaluate the right-hand side of Eq. (3.12). The creation operators c_l^* , with $|l| < n < n^*$, give zero when acting on the state $\exp(-i\sigma G) \mid 0\rangle$, and the commutation relations (3.13) reduce to

$$[\rho_n^+, \psi_+^*(x)] = \exp(-ik_n x)\psi_+^*(x),$$

$$[\rho_n^-, \psi_+^*(x)] = 0.$$
(3.15)

Using Eqs. (2.11) and (3.15) and the definition of $|f_{\sigma}(x)\rangle$, Eq. (3.10), one obtains from Eq. (3.12)

$$\begin{array}{l} (\partial/\partial\sigma) \mid f_{\sigma}(x) \rangle \\ = \exp(i\sigma G) \{ \sum_{n}' \left[\theta(n)/n \right] \exp(-ik_{n}x)\rho_{n}^{-} \} \\ \times \exp(-i\sigma G) \mid f_{\sigma}(x) \rangle, \quad (3.16) \end{array}$$

which is a differential equation for $|f_{\sigma}(x)\rangle$, with the boundary condition

$$|f_0(x)\rangle = \psi_+^*(x) |0\rangle.$$

The commutation relations (3.15) hold in the Luttinger model as operator identities, if one replaces ρ_n^+ , ρ_n^- by ρ_{1n} , ρ_{2n} , and ψ_+^* by ψ_1^* . A differentialequation equivalent to Eq. (3.16) arises there, and the evaluation of I_{++} proceeds from this point exactly like that of I(x, y) in Ref. 6, with the result

$$I_{++} = \langle 0 | \psi_{+}(x')\psi_{+}^{*}(x) | 0 \rangle$$

 $\times \exp\{ \sum_{n>0} (2/n) \sinh^{2}\theta_{n} [\cos k_{n}(x-x')-1] \}.$ (3.17)

The ground-state matrix element is

$$\langle 0 | \psi_{+}(x')\psi_{+}^{*}(x) | 0 \rangle = (1/L) \sum_{n > n \neq r} \exp[ik_{n}(x'-x)].$$

(3.18)

We can immediately write down the expression for I_{-} from Eq. (3.9), and we finally obtain

$$I(x', x) = (1/L) \sum_{n>n_F} \{ \exp[ik_n(x'-x)] + \exp[-ik_n(x'-x)] \}$$
$$\times \exp\{ \sum_{n'>0} (2/n') \sinh^2\theta_{n'} [\cos k_{n'}(x-x')-1] \}, \quad (3.19)$$

or, on replacing the summation over n by integration

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over k,

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$$I(x', x) = \exp\left[-Q(x-x')\right]\pi^{-1}\int_{k_F}^{\infty} \cos k(x-x') dk$$
(3.20)

where

$$Q(x-x') = \sum_{n>0} (4/n) \sinh^2 \theta_n \sin^2 \frac{1}{2} k_n (x-x'). \quad (3.21)$$

Inserting I(x', x) from Eq. (3.20) into Eq. (3.1), we get

$$n(k) = 1 - (\pi L)^{-1} \iint_{-L/2}^{L/2} dx dx' \exp[-Q(x-x')]$$
$$\times \exp[ik(x-x')] \int_{k_F}^{\infty} \cos k'(x-x') dk'. \quad (3.22)$$

This is simplified by noting that Q(0) = 0, so that

$$(\pi L)^{-1} \iint_{-L/2}^{L/2} dx dx' \exp\left[-Q(x-x')\right]$$
$$\times \exp\left[ik(x-x')\right] \int_{0}^{\infty} \cos k'(x-x') dk' = 1.$$

Thus

$$n(k) = (\pi L)^{-1} \iint_{-L/2}^{L/2} dx dx' \exp[-Q(x-x')]$$
$$\times \exp[ik(x-x')] \int_{0}^{k_{F}} \cos k'(x-x') dk'. \quad (3.23)$$

Making the change of variable $x' \rightarrow x-r$, integrating over k' and x, and going to the macroscopic limit N, $L \rightarrow \infty$, we finally obtain

$$n(k) = n^+(k) + n^-(k), \qquad (3.24)$$

where

$$n^{\pm}(k) = \pi^{-1} \int_{0}^{\infty} dr \{ \exp[-Q(r)]/r \} \sin(k_{F} \pm k) r. \quad (3.25)$$

For the noninteracting system, Eqs. (2.12) and (3.21) yield Q(r) = 0, so that n(k) = 0 for $|k| > k_F$ and n(k) = 1 for $|k| < k_F$.

We are now interested in the value of n(k) deep inside the core. Let us take k=0 for convenience:

$$n(0) = (2/\pi) \int_{0}^{\infty} dr \{ \exp[-Q(r)]/r \} \sin k_{F}r. \quad (3.26)$$

The main contribution to this integral comes from the region $r < k_F^{-1}$. We expand Q(r), an even function of r, for small r:

$$Q(\mathbf{r}) \approx \mathbf{r}^2/4b^2, \qquad (3.27)$$

where

or

$$b^{-2} = 4(2\pi/L)^2 \sum_{n>0} \sinh^2 \theta_n.$$
 (3.28)

From Eqs. (3.26) and (3.27) we obtain

 $n(0) = \operatorname{erf}(k_F b).$

Hence, for n(0) to be close to unity, $(k_F b)$ must be large. Using the asymptotic expansion for erf(x), we write

$$n(0) \approx 1 - (\pi^{1/2} k_F b)^{-1} \exp[-(k_F b)^2].$$
 (3.29)

For nonzero values of k deep within the core, the major contribution to the integrals of Eq. (3.25) still comes from the region of small r, so that $n^{\pm}(k)$ is given by

$$n^{\pm}(k) = \frac{1}{2} \operatorname{erf}[(k_F \pm k)b].$$

Defining $\kappa = k/k_F$ and using the same asymptotic expansion for erf(x), we obtain

$$n^{\pm}(k) = \frac{1}{2} - \frac{1}{2} \left[\pi^{1/2} k_F b (1 \pm \kappa) \right]^{-1} \exp\{ - \left[(1 \pm \kappa) k_F b \right]^2 \}.$$
(3.30)

Note that this approximation is very good, provided that the magnitude of $(1\pm\kappa)$ is greater than or of order unity. In particular, for $k\approx k_F$ or $\kappa\approx +1$, the above approximation for $n^+(k)$ is excellent, although the approximation for $n^-(k)$ fails. Thus Eq. (3.30) represents the momentum distribution everywhere except for a narrow interval around k_F .

From Eq. (3.29) it can be seen that the major assumption of the Tomonaga model will be an excellent one, provided that

$$(k_F b)^2 \gg 1$$

$$1 \gg (4/k_F^2) (2\pi/L)^2 \sum_{n>0} n \sinh^2 \! \theta_n$$

Using Eq. (2.12) and setting $k_F = \pi N/L$, we obtain, in terms of the interaction,

$$\frac{1}{16}N^2 \gg \sum' \{ (1 + NJ_n/2\epsilon_F)^{1/2} + (1 + NJ_n/2\epsilon_F)^{-1/2} - 2 \} n.$$
(3.31)

It is interesting to note that this is exactly the condition given by Tomonaga for the applicability of his method, but it was derived by him in a completely different manner. Tomonaga argues that the state with the highest excitation energy, which is compatible with the filled-core assumption, is the state in which all particles in the interval $[|n_F|, |n_F|]$ are excited to single-particle states in the interval $[|n_F|, |n_F+n^*|]$. He then requires that the average excitation kinetic energy per particle be smaller than the excitation energy in this special state and obtains the result of Eq. (3.31). By this reasoning, Eq. (3.31) is only a

necessary condition, while having derived it directly from the momentum distribution function, we have also established its sufficiency. Moreover, the condition of Eq. (3.31) arises because we want the exponentials in Eqs. (3.29) and (3.30) to be small, and this is our primary requirement; while in the Tomonaga treatment, the condition of Eq. (3.31) appears as it stands. If it can be assumed that the error involved in the Tomonaga method is proportional to the number of holes in the core, then the error connected with any acceptable value of the right-hand side of Eq. (3.31) is actually much smaller than implied by Tomonaga's argument.

To obtain a qualitative understanding of Eq. (3.31)in terms of the strength and range of the two-body potential, consider a slowly varying potential of strength V and range R. The Fourier components of such a potential can be approximated by

$$J_n = VR/L \quad \text{for } |n| < n_R = L/R$$
$$= 0 \quad \text{otherwise}$$

As previously noted, it is essential for the Tomonaga method that $n_R \ll n_F$, which implies

$$R/r_0 \gg 1,$$
 (3.32)

where r_0 is the average interparticle separation L/N. On evaluating Eq. (3.31), one has to distinguish between repulsive and attractive interactions. In the former case, the first term on the right-hand side of Eq. (3.31) is dominant, while in the latter case it is the second term which may become prohibitively large. Keeping this in mind, we obtain, after some simple manipulations,

$$(R/4r_0)^3 \gg V/2\epsilon_F \tag{3.33}$$

for repulsive interactions and

$$1-4(2r_0/R)^4 \gg |V|R/2r_0\epsilon_F$$

for attractive interactions. Because of Eq. (3.32), this last inequality may be written as

$$r_0/R \gg |V|/2\epsilon_F. \tag{3.34}$$

For repulsive interactions, one sees that the longer the range, the stronger is the permissible interaction. There is practically no limit on the strength of the interaction, provided that the range is sufficiently long. For attractive interactions, on the other hand, a shorter range implies a stronger permissible interaction. In either case, the range of the interaction must be much larger than the average interparticle separation.

The inequality (3.34) expressed in terms of the Fourier components of the interaction potential becomes

$$N \mid J_n \mid / 2\epsilon_F \ll 1 \tag{3.35}$$

for all *n*. Note that this inequality is more restrictive than the weaker inequality (2.13). By examining the energies of the collective modes of oscillation of the system, one can easily show that the weak inequality (2.13) guarantees the stability of the system against collapse under attractive forces.⁹ The content of inequality (3.35) is that it is necessary but not sufficient that the system be stable in order that the use of the Tomonaga model be justified.

We shall next discuss the behavior of the momentum distribution function n(k) near the Fermi energy. For definiteness, we shall consider the region $k \approx +k_F$. Let us mention once more that results qualitatively similar to most of those derived below were obtained in Ref. 7 for the Luttinger model. From Eq. (3.24)

$$n(k) = n^+(k) + n^-(k)$$
.

As noted previously, the approximation of Eq. (3.30) is very good for $n^+(k)$ for $k \approx k_F$, so that $n^+(k)$ is an analytic function of k in the neighborhood of $k=k_F$, and is nearly constant there. Its value at k_F is, from Eq. (3.30) with $\kappa = +1$,

$$n^{+}(k) = \frac{1}{2} - (4\pi^{1/2}k_{F}b)^{-1} \exp[-(2k_{F}b)^{2}]. \quad (3.36)$$

Any discontinuity in the momentum distribution function at $k = k_F$ must come from the function

$$n^{-}(k) = \pi^{-1} \int_{0}^{\infty} \frac{e^{-Q(r)}}{r} \sin(k_{F} - k) r dr. \quad (3.37)$$

The behavior of $n^-(k)$ at $k=k_F$ is clearly determined by the behavior of $\exp[-Q(r)]/r$ for large r. To determine this latter behavior, we rewrite Eq. (3.21) for Q(r), replacing summation over n by integration over k:

$$Q(r) = \int_{0}^{\infty} (4/k) \sinh^{2}\theta(k) \sin^{2}(\frac{1}{2}kr) dk. \quad (3.38)$$

The derivative of Q(r) with respect to r is

$$Q'(r) = 2 \int_0^\infty \sinh^2 \theta(k) \, \sin kr dk.$$

Integrating by parts three times and keeping in mind that J(k) and hence $\sinh^2\theta(k)$ vanish for large k, we find

$$Q'(r) = 2 \sinh^2 \theta(0) / r + 0(1/r^3), \qquad (3.39)$$

which implies

$$Q(\mathbf{r}) \rightarrow 2\sinh^2\theta(0)\,\ln\mathbf{r} + C + 0(1/\mathbf{r}^2) \qquad (3.40)$$

for large *r*. Therefore, the asymptotic behavior of $\exp[-Q(r)]/r$ is

$$\exp[-Q(\mathbf{r})]/\mathbf{r} \rightarrow e^{-C}/r^{1+\lambda}, \qquad (3.41)$$

⁹A similar inequality with the same content arises in the Luttinger model.



FIG. 2. The possible patterns of behavior of n(k) near $k = k_F$.

where

$$\lambda = 2 \sinh^2 \theta(0) \ge 0. \tag{3.42}$$

Note that λ can only equal zero when J_0 , the space integral of the interaction potential, vanishes. In the general case, λ is positive.

Given the behavior expressed in Eq. (3.41), we rewrite $n^{-}(k)$ in the form

$$n^{-}(k) = \pi^{-1} \int_{0}^{N} \{ \exp[-Q(r)]/r \} \sin(k_{F} - k) r dr + (e^{-C}/\pi) \int_{N}^{\infty} \frac{\sin(k_{F} - k) r dr}{r^{1+\lambda}}, \quad (3.43)$$

where N is some large number, independent of k, such that $\exp[-Q(r)]/r$ may be replaced in the interval $[N, \infty]$ by its asymptotic form. The first term is linear in (k_F-k) near $k=k_F$. In the second term we substitute $(k_F-k)r=u$ and write it as

$$\operatorname{sgn}(k_F - k) \mid k_F - k \mid^{\lambda} (e^{-C}/\pi) \int_{|k_F - k|N}^{\infty} (\sin u/u^{1+\lambda}) du.$$
(3.44)

It is easy to show that Eqs. (3.43) and (3.44) imply for $k \approx k_F^{10}$

$$n^{-}(k) = (k_F - k)C_1(\lambda) + \operatorname{sgn}(k_F - k) \mid k_F - k \mid^{\lambda} C_2(\lambda),$$
$$\lambda \neq 2n + 1 \quad (3.45a)$$
$$n^{-}(k) = (k_F - k)C_1(\lambda) + (k_F - k) \ln \mid k_F - k \mid.$$

$$\lambda = 1$$
 (3.45b)

where $C_1(\lambda)$, $C_2(\lambda)$ depend on λ but not on k. The quantity

$$C_2(0) = \frac{1}{2}e^{-C}, \qquad (3.46)$$

where C is the same constant as in Eqs. (3.40) and (3.41), will be of interest to us.

The behavior of the distribution function $n(k) = n^+(k) + n^-(k)$ at the Fermi energy is now completely determined. We consider first the general case for which λ [Eq. (3.42)] is positive. According to Eq. (3.45), $n^-(k)$ is a continuous function of k at $k = k_F$. As $n^+(k)$

is also continuous there, we conclude that the distribution function is continuous at the Fermi energy regardless of the strength of the interaction. The value of $n^{-}(k_F)$ is zero, so that $n(k_F) = n^{+}(k_F)$, which is given by Eq. (3.36). Taking the derivative of Eq. (3.45), we find that the derivative of the distribution function is infinite if $\lambda \leq 1$. In this case the behavior of n(k) at the Fermi energy is determined by the second term of Eq. (3.45), which dominates for small $|k_F - k|$. For $\lambda > 1$, the derivative is finite, and the distribution function is linear at $k = k_F$. There is practically no trace left of the Fermi surface. For attractive interactions, the condition of applicability [Eq. (3.35)], combined with Eqs. (2.12) and (3.42), implies $\lambda < 1$, so that, in this case, the distribution function has an infinite derivative if the Tomonaga model is at all applicable.

Lastly, we consider the special case in which $\lambda = 0$. According to Eqs. (3.45) and (3.46), the distribution function now has a discontinuity¹¹ at the Fermi energy of magnitude e^{-C} . The quantity C, defined implicitly in Eq. (3.40), is determined as a function of the interaction in the Appendix. In the general case, C is given by

$$C = 2 \int_0^\infty k^{-1} [\sinh^2 \theta(k) - \sinh^2 \theta(0) \cos k] dk. \quad (3.47)$$

For the case

$$\lambda = 2 \sinh^2 \theta(0) = 0,$$

in which we are interested,

$$C = 2 \int_{0}^{\infty} \left[\sinh^2 \theta(k) / k \right] dk > 0.$$
 (3.48)

Thus the magnitude of the discontinuity at the Fermi energy decreases with increasing interaction strength.

We have found various patterns of behavior of the distribution function near the Fermi energy, which are illustrated in Fig. 2. It is worth pointing out, in conclusion, that the significance of λ may be understood on physical grounds. It indicates that at the Fermi surface it is only the very-long-range part of the interaction J_0 which counts.

4. SUMMARY

In Sec. 2 we reviewed and compared the Tomonaga and the Luttinger models. The conclusion is that the Luttinger model is not as unphysical as it may appear from first sight. Suitable interpretation shows that it is essentially equivalent to the Tomonaga model.

In Sec. 3 we checked the basic assumption of the Tomonaga model. The number of holes in the core was found to be negligibly small, provided that Eq. (3.31) is satisfied. Since the right-hand side of Eq. (3.31) appears in an exponential, the condition is in fact much weaker than implied by the "much less than" sign. The forces which are generally believed to be involved

¹⁰ Strictly speaking, Eq. (3.45a) is correct only for $\lambda < 3$. For higher λ , new terms appear whenever λ passes an integer 2n+1. These terms cannot be neglected with respect to $|k_F - k| \lambda$. We do not, however, go into such details, because for $\lambda > 1$ the leading term is linear and all other terms can be neglected. The expression (3.45b) for $\lambda = 2n+1(n \ge 1)$ is also modified, but the behavior at $k \approx k_F$ is again determined by the dominant linear term.

¹¹ This possibility was not pointed out explicitly in Ref. 7, although it is implied by formula (77) of that paper.

in superconductivity seem to be of such a strength and range as to satisfy this condition. Although the derivation is valid only for the ground state (at T=0), we can safely assert that thermal excitations at sufficiently low temperatures will have a negligible effect on these results. It thus seems that, as far as the strength and range of the interaction are concerned, the application of the Tomonaga model in Ref. 5 is justified.

In conclusion, we point out that the core $[-n^*, n^*]$ is not completely filled, and it is an open and interesting question to estimate the effect of a few holes present in the core.

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APPENDIX

The quantity C is defined in Eq. (3.40) by the asymptotic behavior of the function Q(r) for large r:

$$Q(r) \xrightarrow{} 2 \sinh^2 \theta(0) \ln r + C + O(1/r^2).$$
(A1)

It is convenient to rewrite $Q(\mathbf{r})$, given in Eq. (3.38), as

$$Q(\mathbf{r}) = \int_{0}^{\infty} \lambda(k) \left(1 - \cos k\mathbf{r}\right) k^{-1} dk, \qquad (A2)$$

where

$$\lambda(k) \equiv 2\sinh^2\theta(k). \tag{A3}$$

Using the relationship

$$\int_0^\infty k^{-1}(\cos k - \cos kr)\,dk = \ln r$$

and Eq. (A3), Eq. (A2) may be written

$$Q(\mathbf{r}) = 2 \sinh^2\theta(0) \ln^2\theta(0)$$

$$+ \int_0^\infty \left[\lambda(k) - \lambda(0) \, \cos k \right] k^{-1} dk - T(r), \quad (A4)$$

where

$$T(\mathbf{r}) = \int_{\mathbf{0}}^{\infty} k^{-1} [\lambda(k) - \lambda(0)] \cos k\mathbf{r} dk.$$

Integrating by parts twice, we find

$$T(r) \rightarrow O(1/r^2) \tag{A5}$$

for large r. Combining Eqs. (A4) and (A5) and comparing with Eq. (A1), we obtain

$$C = \int_{0}^{\infty} k^{-1} [\lambda(k) - \lambda(0) \cos k] dk.$$

Using Eq. (A3) to express this in terms of $\theta(k)$, one obtains Eq. (3.45) of the text.

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Elementary Excitations in fcc Solid Ortho-Hydrogen

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An equation-of-motion formalism is used to give a nonlinear spin-wave treatment of fcc solid orthohydrogen. The elementary excitations in ortho-hydrogen are librational waves and can be treated in a manner similar to spin waves in magnetism. The excitation spectrum, long-range order, and ground-state energy are calculated. It is found that the spin-wave excitations have a nonvanishing effect on both the long-range order and the ground-state energy. But, because of a large energy gap, the spin-wave-theory results deviate only slightly from their molecular-field values.

I. INTRODUCTION

THE cooperative orientational ordering of ortho- H_2 molecules on a rigid fcc lattice has been described in terms of a molecular-field approximation by Raich and James.^{1,2} This treatment was based on a knowledge of the molecular equilibrium orientations, as found from the ground state of a system of classical quadrupoles on

¹ J.C. Raich and H. M. James, Phys. Rev. Letters **16**, 173 (1966). ² H. M. James and J. C. Raich, Phys. Rev. **126**, 649 (1967).