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Theory of the quasi-one-dimensional electron gas with strong "on site" interaction

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A quasi-one-dimensional system with strong attraction between electrons on the same site is analyzed in terms of an equivalent weakly interacting array of Heisenberg-Ising spin chains. The single-chain ground-state properties and elementary excitation spectrum are discussed. It is shown that for certain ranges of the coupling constants, gapless excitations rather widely believed to be present do not in fact exist. Some inadequacies in a recent derivation of a mean-field ordering temperature for interacting spin chains are pointed out, and a new derivation is given. The application of this technique to the quasi-one-dimensional electron system is discussed.

I. INTRODUCTION

Recently, several authors[1-4] have discussed the theory of a one-dimensional gas on a lattice, where the dominant term in the Hamiltonian is an interaction U between electrons occupying the same lattice site. The other terms put into the Hamiltonian are a nearest-neighbor tunneling term T and an interaction V between electrons on neighboring sites. Efetov and Larkin[1] proved that for positive U and for a particular value of V the model was exactly soluble and the asymptotic behavior of the various correlation functions could be deduced from an equivalent free-boson Hamiltonian. They conjectured that this type of equivalence might hold for general values of V. The present author[2] confirmed that conjecture by demonstrating that their Hamiltonian, for general V, was equivalent for long wavelengths to an anisotropic spin chain and hence, following Luther and Peschel,[5] to a free-boson Hamiltonian. Independently, Emery[3] formulated the model and followed a similar path to derive the density-density and superconducting correlation functions. He then applied the mean-field theory of Imry, Pincus, and Scalapino[6] to find possible transition temperatures for a three-dimensional array of chains.

In Sec. II, we analyze the elementary excitation spectrum and the ground-state order for the isolated one-dimensional system. Previous work in this area by Gurgenishvili *et al.*[4] is shown to be based on incorrect results of des Cloiseaux and Gaudin,[7] and yields a qualitatively incorrect picture for V repulsive. Specifically, they claim that gapless density excitations exist in this regime, whereas we shall show that (for V repulsive) the model has no gapless excitations of any kind. Furthermore, they state that the ground state exhibits long-range order only in the infinite V limit—we shall prove that arbitrary small (but positive) V gives ground-state long-range order.

In Sec. III, possible ordering temperatures for a weakly coupled array of one-dimensional systems are discussed. Imry *et al.*[6] have developed a mean-field theory for weakly interacting spin chains, using a "quantum corrected" classical analysis. It is shown that this approach is in fact inadequate in the extreme quantum limit of spins-$\frac{1}{2}$—for example, their expression for the ordering temperature diverges. Nevertheless, using a fully-quantum-mechanical approach,[8] we find that the coupling-constant dependence of their expression for the ordering temperature is correct, and the divergence is eliminated. Furthermore, the result can now be applied to predict transition temperatures in electronic systems. This has already been done by Emery,[3] but is perhaps worth discussing again here because Emery gives no explicit discussion of the validity of the formulas of Imry *et al.* in the quantum regime.

II. ELEMENTARY EXCITATIONS AND GROUND-STATE ORDER IN ONE DIMENSION

In this section, we consider the one-dimensional electron system described by the Hamiltonian

$$H = U\sum n_{i+}n_{i-} + T\sum (a_{i+1}^{\dagger}a_i + a_i^{\dagger}a_{i+1}) + V\sum_{|i-j|=1} n_i n_j \quad , \tag{2.1}$$

where $U<0$ and $|U| >> |T|, |V|$. The basic approximation is to assume U sufficiently large that each site is either unoccupied or doubly occupied. In this case, we can introduce pair operators

$$b_i^{\dagger} = c_{i+}^{\dagger}c_{i-}^{\dagger} \quad , \tag{2.2}$$

and it is straightforward to show that $b_i^{\dagger}$, b_i, and n_i satisfy commutation relations isomorphic with those of spin-$\frac{1}{2}$ operators, that is,

$$b_i^{\dagger} \equiv S_i^{+}, \quad b_i^{-} \equiv S_i^{-}, \quad n_i \equiv S_i^{z} + \tfrac{1}{2} \quad . \tag{2.3}$$

The Hamiltonian (2.1) is then equivalent to a chain of interacting spins

$$H' = \sum_i \left(\frac{2T^2}{|U|} (S_i^x S_{i+1}^x - S_i^y S_{i+1}^y - S_i^y S_{i+1}^y) + V S_i^z S_{i+1}^z \right) . \quad (2.4)$$

Following Emery,[3] we choose units such that $2T^2/|U| = 1$ and put $V + 1 = -J_z$, giving

$$H_1 = -\sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z) . \quad (2.5)$$

It is clear from (2.3) that a charge-density wave (CDW) in the electron gas corresponds to antiferromagnetic ordering of the spins in the z direction, a superconducting state corresponds to ferromagnetic ordering in the x-y plane. Density-density and superconducting correlation functions can be deduced from the appropriate spin-spin correlation functions, as discussed by Emery.[3] The elementary excitations of the gas correspond to spin waves on the chain. We mention here for future use that the Hamiltonian (2.5) is unitarily equivalent to one having the signs of J_x, J_y (here, $J_x = J_y = 1$) reversed. The necessary transformation is a rotation of every other spin by π about the z axis. Thus, known spin-correlation functions for antiferromagnetic x direction ordering of an antiferromagnetically coupled chain can be related to superconductivity in our model.

Before going on to analyze the elementary excitations and ground-state order in detail, it is worth considering a very simple model which correctly predicts many of the features of the ground state and elementary excitations. The model is given by replacing each spin operator in H_1 by the corresponding component of a classical vector of unit length. It is easy to see in this classical model that for $|J_z| < 1$ the ground state is ferromagnetically ordered along some direction in the x-y plane. For $J_z < -1$, the system is antiferromagnetically ordered in the z direction. Note that the $|J_z| < 1$ ground state breaks a continuous symmetry (angle of magnetization in the x-y plane) so we expect excitations of arbitrarily low frequency, corresponding to a slow variation of this angle along the chain. For $J_z < -1$, on the other hand, there is no corresponding continuous symmetry, so all excitations are above some minimum frequency. On quantization, then, one might expect an energy gap for $J_z < -1$, not for $|J_z| < 1$.

In the work of Gurgenishvili *et al.*,[4] the elementary excitation spectrum of the electron gas was analyzed using some spin chain results of des Cloiseaux and Gaudin.[7] Gurgenishvili *et al.* concluded that gapless excitations existed for $J_z < -1$. This is a point of some physical consequence. It would have the effect, for example, of drastically lowering the ordering temperature into a CDW state for a three-dimensional loosely interacting array of one-dimensional electronic systems. The precise result of des Cloiseaux and Gaudin used by Gurgenishvili *et al.* is the statement that for the Hamiltonian (2.5) with $J_z < -1$ (actually the unitarily equivalent system with the signs of J_x, J_y changed), spin excitations having $S_z = \pm 1$ have a gap, those having $S_z = 0$ have no gap. Sutherland[9] mentions, in a footnote, that this contradicts numerical work on short chains by Bonner. A discussion of the technical short-comings of the des Cloiseaux-Gaudin analysis is given in the Appendix. A more recent and correct analysis of the elementary excitation spectrum using the Bethe ansatz has been given by Johnson and McCoy.[10] These authors find a gap for $J_z < -1$, in fact $S_z = 0$ and $S_z = \pm 1$ excitations have the same energy. They do not mention the work of des Cloiseaux and Gaudin.

Unfortunately, the Bethe ansatz analysis is not very transparent physically, so it is perhaps worthwhile summarizing the simple physical arguments against gapless excitations for $J_z < -1$. First, the classical system does not have them (see the discussion above). Second, in the antiferromagnetic Ising limit, an elementary excitation for a system with periodic boundary conditions is given by turning over a block of r spins. If r is odd, $S_z = \pm 1$, if r is even, $S_z = 0$. The energy in each case is concentrated at the ends of the block. It is hard to imagine that this energy depends on S_z, even away from the Ising limit, where the approach is still qualitatively correct. This picture, then, is in accordance with the analysis of Johnson and McCoy that the elementary excitation energies are spin independent.

We turn now to the ground state of the one-dimensional spin system. Contrary to the statement of Gurgenishvili *et al.*,[4] the ground state actually has long-range order for $J_z < -1$, corresponding to a CDW ground state for the one-dimensional electron gas. Following Johnson, Krinsky, and McCoy,[11] we note that for $J_z < -1$ the long-range order of the spin system is equal to that in the Baxter model for $T < T_c$. (The correspondence is $|J_z + 1| \propto T_c - T$.) Transcribing the results from their paper, for J_z close to -1 the long-range order builds up very slowly, being proportional to $\exp[-\pi^2/4(2|J_z + 1|)^{1/2}]$. For large $|J_z|$, the order approaches the Ising limit as $1 - 2/J_z^2$. The gap in the elementary excitation spectrum is approximately $2\pi \exp[-\pi^2/2(2|J_z + 1|)^{1/2}]$ for J_z close to -1, increasing to the Ising value as $|J_z|$ becomes large.

III. THREE-DIMENSIONAL ORDERING OF WEAKLY COUPLED ONE-DIMENSIONAL SYSTEMS

In this section, we discuss possible ordering temperatures for a set of weakly coupled one-dimensional systems. The approach throughout is to represent the

effects of neighboring chains as a mean field, following Imry *et al.*[6] and Emery.[3] We first review the "quantum corrected" classical analysis of Imry *et al.* for weakly coupled spin chains, and show how it breaks down in the extreme quantum limit. We then point out that a fully quantum mechanical analysis can be used to extend the validity of their result considerably[8]—to anisotropic coupled chains of spins-$\frac{1}{2}$, and hence, following Emery,[3] to electronic systems.

The quasi-one-dimensional solid we consider is a weakly coupled set of systems each having the Hamiltonian (2.1). The weak coupling consists of interchain hopping and interaction terms $T_{\text{inter}}, V_{\text{inter}}$. For simplicity, we assume that these act only between sites having the same subscript i and belonging to nearest neighbor chains. Under the transformation to the equivalent spin chain Hamiltonian H_1, these interchain terms go to spin-spin couplings precisely analogous to the intrachain couplings in (2.4).

Hence, we have the interacting spin chains Hamiltonian

$$H_1^{3D} = -\sum_{\lambda}\sum_{i}(S_{i\lambda}^{x}S_{i+1\lambda}^{x} + S_{i\lambda}^{y}S_{i+1\lambda}^{y} + J_z S_{i\lambda}^{z}S_{i+1\lambda}^{z}) - \sum_{\substack{\lambda,\lambda' \\ \text{nearest} \\ \text{neighbors}}}\sum_{i}[J_{\perp x}(S_{i\lambda}^{x}S_{i\lambda'}^{x} + S_{i\lambda}^{y}S_{i\lambda'}^{y}) + J_{\perp z}S_{i\lambda}^{z}S_{i\lambda'}^{z}] \ , \tag{3.1}$$

where λ is a chain index, $J_{\perp x} = 2T_{\text{inter}}^2/|U|$, $J_{\perp z} = -2T_{\text{inter}}^2/|U| - V_{\text{inter}}$.

This Hamiltonian is close to one considered by Imry, Pincus, and Scalapino.[6] They developed a mean-field theory to predict the ordering temperature for the set of weakly interacting antiferromagnetic chains:

$$H_{\text{IPS}} = 2J\sum_{i\lambda}\vec{S}_{i\lambda}\cdot\vec{S}_{i+1\lambda} + 2J_\perp\sum_{i\lambda}\vec{S}_{i\lambda}\cdot\vec{S}_{i\lambda+1} \ . \tag{3.2}$$

However, they considered the case of general spin—indeed, their main emphasis was on quantum corrections to the classical high spin case. We are interested only in the quantum limit of spins-$\frac{1}{2}$ and for this case, as we shall see below, their analysis requires some correction.

The basic idea of Imry *et al.*[6] is that if $J \gg J_\perp$, at the three-dimensional ordering temperature the correlation length along the chain is very large—in the classical limit it is

$$\xi = 2JS(S+1)/kT \ , \tag{3.3}$$

and hence many correlated lengths on a single-chain overlap at least two such lengths on neighboring chains, leading to a greater effective cross linkage, and suppression of fluctuations. Furthermore, fluctuations along the length of the chain are treated exactly, so replacing chain-chain interactions by a mean field appears to be a very reasonable approximation. This assumption leads to the following formula for the Neel temperature

$$2zJ_\perp\chi(T_N) = 1 \ , \tag{3.4}$$

where z is the number of nearest-neighbor chains, and χ is the staggered susceptibility of an isolated chain. Following Imry *et al.*, χ is evaluated in terms of the static correlation function

$$G(r) = \langle S_x(0)S_x(r)\rangle \ , \tag{3.5}$$

using

$$\chi = \frac{1}{kT}\int_0^\infty (-1)^r G(r)\,dr \ . \tag{3.6}$$

In the classical limit,

$$G(r) \cong \tfrac{1}{3}S(S+1)e^{-r/\xi}(-1)^r \ , \tag{3.7}$$

where ξ is given by (3.3). This leads to the following expression for T_N in the classical limit:

$$kT_N/J = (2/\sqrt{3})S(S+1)(2z_\perp J_\perp/J)^{1/2} \ . \tag{3.8}$$

It is argued that quantum corrections introduce a power term into $G(r)$, giving

$$G(r) \cong \tfrac{1}{3}S(S+1)r^{-\lambda}e^{-r/\xi}(-1)^r \ , \tag{3.9}$$

leading to a quantum formula for T_N:

$$kT_N/J = 4S(S+1)[(zJ_\perp/3J)\Gamma(1-\lambda)]^{1/(2-\lambda)} \ . \tag{3.10}$$

Imry *et al.* speculate that this semiclassical formula might have some value even in the spin-$\frac{1}{2}$ case, where $\lambda = 1$ (according to Luther and Peschel[5])—they estimate that for $J_\perp \sim 10^{-3}J$, T_N is suppressed by a factor of 10 from the classical prediction. In fact, a little more care is needed because (3.10) actually predicts T_N to be infinite—$\Gamma(0) = \infty$!

The essential point is that the formula (3.6) for the susceptibility is a classical formula, and replacing $G(r)$ by a quantum correlation function does not necessarily give an adequate quantum expression for χ. This is immediately apparent if one considers how (3.6) is derived. If an infinitesimal staggered field $(-1)^r B(r)S_x(r)$ is applied to the chain, the response of the spin at zero is

$$\mathrm{Tr}e^{-\beta H}S_x(0)/\mathrm{Tr}e^{-\beta H} \ , \tag{3.11}$$

where

$$H = H_0 + H_{\text{int}} \ ,$$

and

$$H_{\rm int} = \int (-1)^r B(r) S_x(r)\, dr \quad . \tag{3.12}$$

The classical result (3.6) is given by expanding (3.11) to first order in the small field $B(r)$. For the quantum mechanical case, this expansion is invalid because H_0, $H_{\rm int}$ do not commute. It is necessary therefore to use the standard trick of expanding $e^{-\beta H}$ as a series of time-ordered products of $H_{\rm int}$ in the interaction representation on the imaginary time axis $(0, i\beta)$. For our purposes, we need only the first term in the standard expansion, giving

$$\chi = \int_0^{1/T} d\tau \int_0^{\infty} (-1)^r G(r,\tau)\, dr \quad , \tag{3.13}$$

where $G(r,\tau)$ is the analytic continuation of the time-dependent spin-spin correlation function to imaginary time. According to Luther and Peschel[12]

$$G(r,\tau) \approx [1/(r^2 + c^2\tau^2)]^{1/2} \tag{3.14}$$

for the (isotropic) spin-$\frac{1}{2}$ chain at zero temperature (putting their cutoff α equal to one lattice spacing, our distance unit), the velocity c is of order unity. At nonzero temperatures, an exponential cutoff takes place at large distances, governed by a term of the form $\mathrm{csch}\pi(t - x/c)T$. Inserting this and (3.14) into (3.13), we observe that the integral is cutoff in both the x and τ directions at $\sim T^{-1}$. For an estimate of its value, we can take a cutoff at T^{-1} radially in the x, τ plane. Apart from numerical factors this leads to

$$kT_N/J \sim J_\perp/J \tag{3.15}$$

in essential agreement with Eq. (9) of Imry *et al.*

Therefore, we conclude that, remarkably, the classical formula of Imry *et al.* is essentially correct—that is to say, it correctly predicts the coupling-constant dependence of the transition temperature. The logarithmic divergence given by the classical formulation is eliminated in the quantum version.

We turn now to an application of these ideas to the anisotropic model described by the Hamiltonian (3.1) and the corresponding electron gas system. For the range of parameters $-1 < J_z/J_x < 0$, the two possible types of ordering in a quasi-one-dimensional system are z-direction antiferromagnetic ordering (corresponding to a CDW) and x-direction ordering (superconductivity). The relevant correlation functions[5] are

$$\langle S^z S^z \rangle \sim [1/(r^2 + c^2\tau^2)]^{\theta - 1/2} \quad ,$$
$$\langle S^x S^x \rangle \sim [1/(r^2 + c^2\tau^2)]^{\theta/2} \quad , \tag{3.16}$$

where $\theta = \frac{1}{2} - \pi^{-1}\arcsin J_z$.

Following Emery,[3] these correlation functions can be inserted into (3.13) to give a prediction for the ordering temperature of the form (3.10), with some differing overall numerical factors. Note that it is essential to use the *quantum* formula (3.13)—since $\theta < 1$, the static z-direction correlation function $\sim r^{-\theta^{-1}}$ from (3.16), and inserting this into the classical formula (3.6) gives a divergence worse than that of Imry *et al.* This point is not clearly made in Emery's paper.

Finally, we consider three-dimensional ordering of chains having intrachain coupling with $J_z < -1$. This corresponds to a repulsion between nearest-neighbor sites for the electron gas model. Little is known about the spin-spin correlation function in this case, but some conclusions can be drawn from a knowledge of the corresponding sector of the Baxter model. As mentioned at the end of Sec. II, the single chain has CDW long-range order in the ground state, although for J_z close to -1 the amplitude is exponentially small, and the transition temperature as predicted by the mean-field approach is therefore close to that for the isotropic case. As $|J_z|$ increases further, however, the picture changes drastically. As mentioned in Sec. II, the long-range order rises to the Ising limit as $1 - J_z^{-2}$, so for $|J_z| \geq 2$ it becomes reasonable to use the results of Scalapino, Imry, and Pincus[13] for weakly interacting *Ising* chains to estimate T_N. The result is

$$T_N \simeq \frac{2|J_z|}{\ln|J_z/(J_\perp)_z|} \quad .$$

For large values of $|J_z/(J_\perp)_z|$ this ordering temperature is much higher than even the classical result (3.8) as we expect.

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APPENDIX

In this Appendix we pinpoint the error in des Cloiseaux and Gaudin[7] which we believe invalidates their conclusions concerning the $S_z = 0$ excitations for $J_z < -1$. From Bethe's ansatz[14,15] any state of the antiferromagnetic linear chain can be specified by a set of quantum numbers $\{\lambda_j\}$, where $\lambda_1 < \lambda_2 < \cdots < \lambda_l$. The λ_j's lie between 1 and N (the number of sites) and the number of λ_j's equals the number of up-spins, which we take $\leq \frac{1}{2}N$. An integral equation gives a set of "spin-wave" momentum numbers $\{k_j\}$ from which the total momentum and energy of the state can be deduced. If $|\lambda_j - \lambda_{j+1}| \geq 2$ for all j, the k_j are all real. Otherwise, complex k_j appear. Bethe's

ansatz for the ground state has two possible sets of λ's: $1, 3, \ldots, N-1$ or $0, 2, \ldots, N-2$ $(0 \equiv N)$.

To generate a low-lying excited state, it is natural to try a set of λ's with a gap, des Cloiseaux and Gaudin use

$$\lambda_\alpha = 2\alpha - 2, \quad 1 \leq \alpha \leq n \ ,$$

$$\lambda_\alpha = 2\alpha - 1, \quad n < \alpha \leq \tfrac{1}{2}N \ ,$$

[their Eqs. (109) and (110)]. In the limit of large N, this distribution of λ's is put into an integral equation to generate a distribution of k's, $k(x)$, on the real line. However, the set of λ's used does not satisfy $|\lambda_i - \lambda_{i+1}| \geq 2$ because both zero $(\equiv N)$ and $N-1$ are included. Therefore, the set of k_i's will include complex ones, and the procedure of finding a real distribution $k(x)$ is invalid. For $S_z = 1$ excitations, on the other hand, the quantum number $\lambda_1 = 0$ is omitted, giving a set of λ's corresponding to real k's, so the procedure is valid.

As a final note, we might mention that ignoring the proximity of $N-1$ and 0 (mod N) is something of a tradition in the field. Orbach[14] following the early sections of Bethe's first paper[15] included this pair of numbers in the category of two spin-wave excitations corresponding to real k, thereby overcounting the number of states in this category by one. Bethe, however, corrected himself in a footnote later in the paper, and in his article[16] counted correctly from the start.

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