Spin-correlation effects in a one-dimensional electron gas

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The Singwi-Sjölander-Tosi-Land (SSTL) approach is generalized to study the spin-correlation effects in a one-dimensional (1D) electron gas. It is shown that the SSTL approach yields different and interesting results compared with the more widely used Singwi-Tosi-Land-Sjölander (STLS) approach. We find out that the self-consistent field approaches, STLS and SSTL, predict a Bloch transition for 1D electron-gas systems at low electron densities.

DOI: 10.1103/PhysRevB.70.235305

PACS number(s): 73.21.Hb, 71.45.Gm

I. INTRODUCTION

The Singwi-Tosi-Land-Sjölander (STLS) approach¹ is a powerful theoretical tool in going beyond the random-phase approximation (RPA) in studying the short-range correlation effects of an interacting electron gas. It was originally developed for three-dimensional (3D) electron gas. In the STLS approach the short-range correlation effects are described by a local-field correction in the density response function. The STLS approach is later applied to the two-dimensional $(2D)^{2-4}$ and one-dimensional $(1D)^{5-7}$ electron-gas systems with long-range Coulomb or short-range interactions. The STLS approach gives correct pair-correlation function, but it fails to satisfy the compressibility sum rule.

The Lobo-Singwi-Tosi (LST) approach,⁸ on the other hand, was originally developed to calculate the spincorrelation effects in the 3D interacting electron gas. Although the calculated spin susceptibility is not in agreement with experiment, the LST approach is applied to the $2D^{9-11}$ and $1D^{12,13}$ electron-gas problems.

In this paper, we study the validity of another attempt to go beyond RPA, the Singwi-Sjölander-Tosi-Land (SSTL) approach.^{14,15} It was proposed as an improvement over the STLS approach to better take into account the compressibility sum rule. This sum rule requires that the compressibility computed via the ground-state energy and the longwavelength limit of the static dielectric function of the system be the same. The compressibility sum rule thus requires that at long wavelengths the exact screened density response function, and hence the local-field correction, is determined by the isothermal compressibility. For a review of the STLS, SSTL, and LST approaches see Ref. 16. It is curious that, although it is not very widely used, the SSTL approach was not investigated before for a low-dimensional electron-gas problem. It is therefore of interest to study the SSTL approach, to investigate its range of validity, and to compare its results with the very widely used STLS approach. This is done in our recent work¹⁷ for density correlations in a 1D electron gas. In that work, we showed that the SSTL satisfies the compressibility sum rule better than the STLS approximation.

Our main motivation for studying the spin-correlation effects in 1D electron-gas systems is that these effects are considered to explain the so-called 0.7 structure, and may lead to a phase transition from the paramagnetic to the ferromagnetic state.

In some recent experiments^{18–22} carried with very clean 1D channels, in addition to the usual quantized conductance plateaux, a clear plateaulike structure close to $0.7(2e^2/h)$ has been observed at zero magnetic field. Thomas *et al.*¹⁹ made measurements with six 1D constrictions, which are fabricated from 2D electron gases formed in modulation-doped GaAs/Al_{0.33}Ga_{0.67}As heterostructures grown by molecularbeam epitaxy (MBE) on a (100) semi-insulating GaAs substrate, and in all of the samples investigated they observed clean quantized conductance plateaux as well as the 0.7 structure. It is shown that the 0.7 structure observed in these experiments is not due to transmission or resonance effects. Moreover, the Tomanaga-Luttinger theory or a simple spin polarization of the electron gas cannot describe the origin of this unique structure.

Using the density-functional theory, Wang and Berggren²³ solved the Kohn-Sham equation self-consistently for an infinite quasi-1D channel with an in-plane magnetic field parallel to the channel. The results show that full spin polarization appears at low electron densities ($\sim 10^5 \text{ cm}^{-1}$). Moreover, the results are consistent with observations of the 0.7 structure and its interpretation in terms of spontaneous spin polarization of the lowest subband. Obviously, whether the 0.7 structure reflects spontaneous spin polarization, or other manybody effects, is a topic of considerable current debate. It is therefore interesting to investigate the spin-correlation effects in a quasi-1D electron system within the SSTL approximation, which has not been done before.

The organization of the paper is as follows. In Sec. II we present the formalism and the SSTL approach. Our results and performance of the SSTL approach are discussed in Sec. III.

II. FORMALISM

The ground state of a noninteracting electron gas is paramagnetic. Therefore, the magnetic moments of the constituents are randomly distributed and their magnetic moment is averaged to zero. If we apply a weak external magnetic field to such a system, it will develop a paramagnetic spin moment. The response of the system to the field can be studied via its wave-vector- and frequency-dependent paramagnetic susceptibility function. On the other hand, in an interacting electron system we have short-range exchange and correlation effects. In this study, we investigate these effects within the self-consistent field approximation (SCFA) as in the case of density-density correlations. It is assumed that the electrons are embedded in a uniform positive background so that the whole system is neutral. For ease of notation we will set $\hbar = 1$ throughout this paper.

In the SCFA the wave-vector- and frequency-dependent density and spin-density response functions $\chi^d(q,\omega)$ and $\chi^s(q,\omega)$, respectively, are given by

$$\chi^{d}(q,\omega) = \frac{\chi_{0}(q,\omega)}{1 - \psi^{s}(q)\chi_{0}(q,\omega)},\tag{1}$$

$$\chi^{s}(q,\omega) = -g^{2}\mu_{B}^{2}\frac{\chi_{0}(q,\omega)}{1-\psi^{a}(q)\chi_{0}(q,\omega)},$$
(2)

where $\chi_0(q, \omega)$ is the free-electron polarizability, $\psi^s(\psi^a)$ is the spin-symmetric (antisymmetric) effective potential, *g* is the Landè factor, and μ_B is the Bohr magneton.

The system responds to the applied magnetic field through the free particle susceptibility modified by a local-field correction. The static structure factor S(q) and magnetic structure factor $\tilde{S}(q)$ are related to the dynamic response functions by the fluctuation-dissipation theorem as

$$S(q) = -\frac{1}{n\pi} \int_0^\infty d\omega \operatorname{Im}\{\chi^d(q,\omega)\},\tag{3}$$

$$\widetilde{S}(q) = \frac{1}{n\pi g^2 \mu_B^2} \int_0^\infty d\omega \,\operatorname{Im}\{\chi^s(q,\omega)\},\tag{4}$$

where *n* is the 1D electron-gas density. The Fermi wave number k_F is related to the linear electron density as $n = g_s g_v k_F / \pi$, with g_s and g_v as the spin and valley degeneracy, respectively. In this paper, we take $g_v = 1$, which is the case for GaAl/AlGaAs-based quantum wire structures. The system is characterized by a dimensionless interaction parameter r_s , defined as the ratio of the interelectron spacing to the effective Bohr radius. The r_s is related to the linear electron density as $r_s = 1/(2na_B^*)$, where $a_B^* = \epsilon_0/(e^2m^*)$ is the effective Bohr radius with background dielectric function ϵ_0 and effective electron mass m^* .

In the SCFA the effective potentials $\psi^{s}(q)$ and $\psi^{a}(q)$ are defined as

$$\psi^{s}(q) = V(q)[1 - G(q)], \quad \psi^{a}(q) = V(q)I(q),$$
 (5)

where V(q) is the 1D Fourier transform of the Coulomb potential, and G(q) and I(q) are the static local-field corrections arising from the short-range exchange and correlation effects for the density and spin-density responses, respectively. In the SSTL approximation they are given by

$$G(q) = -\frac{1}{n} \int \frac{dq'}{2\pi} \frac{q'}{q} \frac{V(q')}{\epsilon(q')V(q)} [S(q-q') - 1], \quad (6)$$

$$I(q) = \frac{1}{n} \int \frac{dq'}{2\pi} \frac{q'}{q} \frac{V(q')}{\epsilon(q')V(q)} [\widetilde{S}(q-q') - 1], \qquad (7)$$

where $\epsilon(q)$ is the static dielectric function of the electron gas, which is related to the density response function $\chi^d(q)$ as

$$\frac{1}{\epsilon(q)} = 1 + V(q)\chi^d(q).$$
(8)

In the STLS approach, the potential under the integral sign in Eqs. (6) and (7) is not screened by $\epsilon(q)$.

We model the 1D electron gas as obtained from the zerothickness 2D electron gas under a harmonic confinement potential.²⁴ The electrons are assumed to occupy only the lowest subband. This model yields the Coulomb interaction potential between electrons as $V(q) = (e^2/\epsilon_0)F(q)$, where $F(q) = \exp(x)K_0(x)$ and $x = b^2q^2/4$ with *b* as the lateral width of the quantum wire.

The RPA describes the dielectric properties of the electron gas at high electron densities. In RPA the short-range correlations are assumed to be absent, i.e., the local-field correction G(q)=0. As the density of the system is lowered, the exchange and correlation effects become important. The Hubbard approach (HA) was developed to improve the RPA by introducing a local-field correction which takes into account only the exchange hole around an electron. In the HA, the local-field correction for spin correlations is given by

$$I_H(q) = -\frac{1}{2} \frac{V(\sqrt{q^2 + k_F^2})}{V(q)}.$$
(9)

The spin-symmetric and spin-antisymmetric paircorrelation functions g(r) and $\tilde{g}(r)$, respectively, are related to the static structure factor and magnetic structure factor by a Fourier transform

$$g(r) = 1 + \frac{1}{2} \int_0^\infty dq \, \cos(qr) [S(q) - 1], \qquad (10)$$

$$\widetilde{g}(r) = \frac{1}{2} \int_0^\infty dq \, \cos(qr) [\widetilde{S}(q) - 1]. \tag{11}$$

These may be written in terms of the parallel spin-paircorrelation function $g_{\uparrow\uparrow}(r)$ and antiparallel spin-paircorrelation function $g_{\uparrow\downarrow}(r)$ as

$$g(r) = \frac{1}{2} [g_{\uparrow\uparrow}(r) + g_{\uparrow\downarrow}(r)], \quad \tilde{g}(r) = \frac{1}{2} [g_{\uparrow\uparrow}(r) - g_{\uparrow\downarrow}(r)].$$
(12)

The spin-dependent potentials may be obtained by combining $\psi^{s}(q)$ and $\psi^{a}(q)$ in the following form

$$\psi_{\uparrow\uparrow}(q) = \psi^{s}(q) + \psi^{a}(q), \quad \psi_{\uparrow\downarrow}(q) = \psi^{s}(q) - \psi^{a}(q). \quad (13)$$



FIG. 1. The magnetic structure factor $\tilde{S}(q)$ in the SSTL (solid line), STLS (dashed line), and Hubbard (dotted line) approximations at $r_s=1$ for a quantum wire width of $b=2a_B^*$.

The excitation spectrum ω_q of the collective spin modes are obtained by the poles of the spin susceptibility function $\chi^s(q,\omega)$ as

$$\omega_q = \left(\frac{\omega_-^2 - \omega_+^2 e^{A(q)}}{1 - e^{A(q)}}\right)^{1/2},\tag{14}$$

where $\omega_{\pm} = |q^2/2m^{\star} \pm qk_F/m^{\star}|$ are the boundaries of the particle-hole continuum, and $A(q) = \frac{\pi^2 q}{[4r_s F(q)I(q)]}$.

Spin-density susceptibility of the 1D electron gas in the SCFA may be given by

$$\chi^{s}(q) = \frac{g^{2} \mu_{B}^{2} \rho(\varepsilon_{F}) k_{F}}{q} \frac{\ln \left| \frac{q + 2k_{F}}{q - 2k_{F}} \right|}{1 + \frac{8r_{s}k_{F}}{\pi^{2}q} F(q) I(q) \ln \left| \frac{q + 2k_{F}}{q - 2k_{F}} \right|},$$
(15)

where $\rho(\varepsilon_F) = 2m^* / \pi k_F$ is the density of states at the Fermi energy in 1D electron gas. Note that the Pauli spin susceptibility is $\chi_{Pauli} = \mu_B^2 \rho(\varepsilon_F)$.²⁵



FIG. 2. The change of the critical density parameter r_{sc} with quantum wire width *b* within the STLS approximation.



FIG. 3. The static structure factor S(q) for quantum wire width $b=2a_B^*$ in the SSTL approximation at $r_s=0.5$, 1, and 1.5.

The ground-state energy is the most important physical property in determining the phase of a system. The ground-state energy per particle ϵ_g of a 1D electron-gas system is given by



FIG. 4. The spin-dependent pair-correlation functions (a) $g_{\uparrow\downarrow}(r)$ and (b) $g_{\uparrow\downarrow}(r)$ calculated in the SSTL approximation at $r_s=0.5$ (solid line), $r_s=1$ (dashed line), and $r_s=1.5$ (dotted line) for $b=2a_B^*$.



FIG. 5. The (a) spin-symmetric and (b) spin-antisymmetric effective potentials in the SSTL approximation (solid line), STLS approximation (dashed line), and HA (dotted line) at $r_s=1$ and $b = 2a_B^*$.

$$\varepsilon_{g}(r_{s})/Ry^{\star} = \frac{\pi^{2}}{12g_{s}^{2}g_{\nu}^{2}r_{s}^{2}} + \frac{1}{2r_{s}g_{s}g_{\nu}} \times \int_{0}^{1} d\lambda \int_{0}^{\infty} dq \ F(q)[S(q,\lambda) - 1], \quad (16)$$

where $Ry^* = 1/(2a_B^{*2}m^*)$ is the effective Rydberg and λ is the coupling constant. In this relation the first term is the kinetic energy and the second term is the exchange-correlation energy of the system. Also note that here we normalized the wave number by k_F .

III. RESULTS AND DISCUSSION

The results presented in this section are obtained by solving Eqs. (1)–(4), (6), and (7) self-consistently. In Fig. 1, we present the magnetic structure factor $\tilde{S}(q)$ in different approaches at $r_s=1$. It seems that the Hubbard approximation has the most pronounced peak at $q=2k_F$, whereas the sharpness of the SSTL peak comes out to be the least. We could not obtain $\tilde{S}(q)$ for $r_s > 1.8$, even after 1000 iterations, within the STLS approach. This r_s value corresponds to $n \approx 3$ $\times 10^5$ cm⁻¹ for GaAl/AlGaAs-based quantum wire struc-



FIG. 6. The spin-dependent effective potentials in the SSTL (solid line) and STLS (dashed line) approximations at $r_s=1$ and $b=2a_{R}^{*}$.

tures. It seems that an instability in the paramagnetic phase sets in at this r_s value, as observed in earlier STLS studies.^{12,13} This unfortunately means that we are unable to study different possible phases of the 1D electron gas as one varies the density or equivalently r_s . Similar instability in $\tilde{S}(q)$ has also been observed in 2D electron-gas systems.^{9–11} Moreover, for a 2D electron gas the peak appearing in $\tilde{S}(q)$ calculated within the HA is the highest we observe in a 1D system. It is interesting to observe that the SSTL approach no longer gives a peak in $\tilde{S}(q)$ after $r_s=1.1$. This result must be due to the use of the screened potential in the SSTL approach instead of the bare Coulomb interaction potential as in the STLS.

The change of the critical interaction parameter r_{sc} , where the instability in the unpolarized 1D electron gas appears, with quantum wire width *b* within the STLS approach is plotted in Fig. 2. Obviously, there is no linear relation between r_{sc} and *b*.

In contrast to $\tilde{S}(q)$, the static structure factor S(q) is easier to obtain even for larger values of r_s . The S(q) computed within the SSTL approach for different r_s values is shown in Fig. 3. The SSTL S(q) does not have a peak as $\tilde{S}(q)$, and behaves like other S(q) results.



FIG. 7. The paramagnon dispersion ω_q in the SSTL (solid line) and STLS (dashed line) approximations at $r_s = 1.5$ and $b = 2a_B^*$.

The spin-dependent pair-correlation functions $g_{\uparrow\uparrow}(r)$ and $g_{\uparrow\downarrow}(r)$ calculated within the SSTL approach are shown in Fig. 4 for different electron densities. We notice that $g_{\uparrow\uparrow}(r)$ has a weak r_s dependence and its value at zero separation decreases with increasing r_s . We found that the zero separation value of the spin-independent pair-correlation function g(r) becomes negative for $r_s > 2.1$.¹⁷ Since g(r) is the probability of finding an electron at a distance r when another electron is located at origin, negative g(0) is a drawback of the SSTL approach. It should also be noted that the SSTL approach gives negative values for g(0) in 3D electron gas.^{14,15} Negative g(0) is the price that we have paid for satisfying the compressibility sum rule better.

The spin-symmetric and spin-antisymmetric effective potentials $\psi^{s}(q)$ and $\psi^{a}(q)$, respectively, in units of V(q) computed within different approximations are shown in Fig. 5. We notice that although the HA and STLS results are rather similar, the SSTL result has a different behavior. The SSTL $\psi^{a}(q)$ starts from a slightly positive value and, after a little increase for small q range, it decreases and finally reaches a value closer to the HA result at large q. Our STLS and HA results are in good agreement with those of Ref. 12.



FIG. 8. The static spin response function $\chi^{s}(q)$ in the SSTL (solid line) and STLS (dashed line) approximations at $r_{s}=1$ and $b=2a_{B}^{\star}$.



FIG. 9. The ground-state energy per particle of the paramagnetic (solid line) and ferromagnetic (dashed line) phases calculated within the SSTL and STLS approximations for $b=2a_B^*$.

The results for the spin-dependent potentials $\psi_{\uparrow\uparrow}(q)$ and $\psi_{\uparrow\downarrow}(q)$ at $r_s=1$ in SSTL and STLS approaches are compared in Fig. 6. We find that $\psi_{\uparrow\uparrow}(q)$ is less than $\psi_{\uparrow\downarrow}(q)$ for the same r_s value. This is an expected result because the charge depletion is more for a pair of electrons with parallel spins than that with antiparallel spins. It is also observed that $\psi_{\uparrow\uparrow}(q)$ is slightly negative at large q values in the SSTL. We therefore conclude that the short-range correlations are overestimated in the SSTL approach. According to the Pauli exclusion principle, $\psi_{\uparrow\uparrow}(q)$ must tend to zero as $q \to \infty$. Negative $\psi_{\uparrow\uparrow}(q)$ at large q values is also observed in the SCFA calculations done for 2D electron gas.⁹

The wave-vector dependence of the paramagnon frequency ω_q is found by the complex poles of $\chi^s(q, \omega)$. In Fig. 7 we present ω_q at $r_s=1.5$ computed within the SSTL and STLS approximations for comparison. We notice that the SSTL ω_q is larger than the STLS value. In both approaches ω_q shows a linear behavior for small q, as observed before.¹²

The static spin susceptibility of the 1D electron system in our model is computed by using Eq. (15). In Fig. 8 we show $\chi^{s}(q)$ for $r_{s}=1$ in both SSTL and STLS approaches. We notice that $\chi^{s}(q)$ has a singularity at $q=2k_{F}$ due to the freeelectron susceptibility $\chi_{0}(q)$, which shows a logarithmic divergence at $q=2k_{F}$. It is seen that the results in both approaches are qualitatively and quantitatively similar. The peak at $q=2k_F$ is less pronounced in the SSTL approach, which seems to be its dominant character.

We plot the ground-state energy per particle results up to $r_s=5$ in both paramagnetic and ferromagnetic phases, $g_s=2$ and 1, respectively, within the SSTL and STLS approaches in Fig. 9. It seems that the ferromagnetic phase becomes energetically favorable after around $r_s=2$. This result was reported for a 1D electron-gas system interacting via a potential, which is slightly different than the one we employ within the STLS approach.^{13,26} The transition from an unpolarized to a polarized system in an electron gas due to the many-body effects is called the Bloch transition.²⁷ According to the Lieb-Mattis theorem²⁸ the ground state of N electrons in 1D subject to an arbitrary symmetric potential must be unmagnetized, or paramagnetic. However, the theorem does not apply to electrons in 3D interacting via Coulomb or central forces, because such potentials are not separately symmetric. In our calculations, we considered that the electrons interact via Coulomb potential. Hence, the Lieb-Mattis theorem should not be applicable to our problem. Also, it is proposed by Calmels and Gold¹³ that for $r_s \ge r_{sc}$ the system might still be unmagnetized but the spin degeneracy is lifted. On the other hand, in a recent quantum diffusion Monte Carlo study²⁹ the energies are found to be in the same order imposed by the Lieb-Mattis theorem.

The most important difference observed in Fig. 9 is that the energy difference between the paramagnetic and ferromagnetic phases increases with increasing r_s in favor of the ferromagnetic phase in the SSTL approach. On the other hand, within the STLS approach the energies in both phases remain close to each other as r_s increases.

In summary, we have studied the spin correlations in a 1D electron system in detail and have shown that the SSTL approach yields different results compared with those obtained within the STLS approach. For example, in the STLS approach the magnetic structure factor $\tilde{S}(q)$ shows a peak at some critical density, beyond which we could not compute the $\tilde{S}(q)$, whereas the SSTL approach gives no peak in the $\tilde{S}(q)$ as we lower the density. It is also observed that the short-range correlations are overestimated, and the energy of the collective spin modes is higher in the SSTL approach. Moreover, the ground-state energy difference between the paramagnetic and ferromagnetic states at the same density is larger in the SSTL approach.

The most important finding of this work is that the selfconsistent field approaches STLS and SSTL predict the Bloch transition for 1D electron-gas systems at low electron densities.

ACKNOWLEDGMENT

We thank Dr. C. Bulutay for useful discussions.

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