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Many-body effects in the one-dimensional electron gas with short-range interaction: the Singwi, Tosi, Land and Sjölander approach including spin polarization

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Received 1 December 1997

Abstract. We study many-body effects in the one-dimensional electron gas and a repulsive delta-function interaction potential (of strength V_0) using the STLS approach. The STLS approach is *generalized* in order to treat polarization effects. We present numerical results for the compressibility and the spin susceptibility and we compare with the quasi-exact analytical result. The validity range of the STLS approach is characterized by $\gamma_{HFA} = \pi^2/2$ with $\gamma = mV_0/N$, where *m* is the electron mass and *N* the electron density.

1. Introduction

The Singwi, Tosi, Land and Sjölander (STLS) approach [1] is a powerful approximating theory for calculating the ground-state energy (GSE) and the compressibility of the interacting electron gas. In this paper we generalize the STLS approach in order to study polarization effects and the spin susceptibility of the one-dimensional electron gas with a short-range interaction potential. We compare our results with quasi-exact calculations and determine the validity range of the generalized STLS approach.

The STLS approach was originally developed for the three-dimensional electron gas with long-range Coulomb interaction. It is well known that this approach gives quite good results as regards the ground-state energy and the compressibility. The Lobo, Singwi and Tosi (LST) approach [2] was developed to calculate spin-correlation effects in the interacting electron gas. In the STLS approach and the LST approach many-body effects are described by the local-field correction for the density-response function and the spin-response function, respectively. However, it was found that the spin susceptibility obtained within the LST approach is not in agreement with experiment. Nevertheless, this approach has been applied to the two-dimensional and one-dimensional electron gas with long-range Coulomb interaction [3]. For a review of the STLS and the LST approaches, see reference [4].

In this paper we study a one-dimensional electron gas with a short-range interaction potential. This model was introduced previously [5] and the exact GSE was calculated as a function of the interaction strength parameter [6]. The STLS approach was applied to this model [6]; however, only the GSE was calculated. In a recent paper [7] we used the STLS

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approach and the LST approach, and obtained analytical results for the local-field correction (LFC) for weak and strong coupling. In the present paper we calculate the compressibility and the spin susceptibility by using a generalized STLS approach. The generalized STLS approach is obtained by introducing spin-polarization effects into the STLS approach. It was introduced recently to calculate the spin susceptibility of a quasi-one-dimensional electron gas with long-range Coulomb interaction [8]. We compare our results with quasi-exact results for this model obtained by means of a ladder calculation [9] and we determine the validity range of the STLS approach. This is an important topic because the STLS approach and the LST approach are widely used. In fact, we show that the STLS approach gives, for the compressibility and the spin susceptibility, quite reasonable results up to a large interaction strength parameter.

The paper is organized as follows. In section 2 we present the model and the theory. The results for the GSE are described in section 3. The compressibility is calculated in section 4 and the spin susceptibility is derived in section 5. A discussion of our results is given in section 6. We give our conclusions in section 7.

2. Model and theory

The model is a one-dimensional electron gas with kinetic energy (characterized by an effective mass m and by a parabolic dispersion $\varepsilon(q) = q^2/2m$ and an interaction energy characterized by the potential V_0 . The wire axis is supposed to be in the z-direction. The interaction potential is a short-range potential of the form $V(r) = V_0 \delta(r)$ and r is the distance between two electrons. The Fourier transform of the interaction potential is given by $V(q) = V_0$. In terms of the electron density N, the electron mass, and the strength of the interaction, we define the dimensionless interaction strength parameter γ as $\gamma = mV_0/N$. The electron density determines the Fermi wavenumber k_F via $N = 2k_F/\pi$. With $v_F = k_F/m$ as the Fermi velocity, the interaction strength parameter is given by $\gamma = \pi V_0/2v_F$. Using the density of states $\rho_F = N/2\varepsilon_F$ at the Fermi energy ε_F , one can write $V_0 \rho_F = 4\gamma/\pi^2$. The spin-polarization parameter ξ with $0 \leq |\xi| \leq 1$ is given by $\xi = (N_+ - N_-)/N$ with $N = N_+ + N_-$. The electron densities N_{\pm} are expressed as $N_{\pm} = N(1 \pm |\xi|)/2$. The Fermi wavenumbers for the polarized subsystems are written as $k_{F\pm} = k_F(1\pm |\xi|) = \pi N_{\pm}$. The essential parameters of the theory are N and ξ for the electron gas and γ for the interaction. We express all of the results as functions of γ and ξ and we use $h/2\pi = 1$.

For a short-range interaction potential, the LFC within the STLS approach is independent of the wavenumber [6], and the dynamic density-response function $X(q, \omega)$ is given by

$$X_0(q,\omega) = \frac{X_0(q,\omega)}{1 + V_0[1 - G(\gamma,\xi)]X_0(q,\omega)}.$$
(1)

 $X_0(q, \omega)$ is the Lindhard function of the one-dimensional free-electron gas. $G(\gamma, \xi)$ is the LFC for density fluctuations and $G(\gamma, \xi = 0)$ was discussed before [7]. Within the STLS approach the LFC is given by [6]

$$G(\gamma,\xi) = \frac{1}{\pi N} \int_0^\infty dq' \ [1 - S(q',\gamma,\xi)].$$
(2)

 $S(q, \gamma, \xi)$ is the static structure factor (SSF) and we use, following the arguments given in [7, 8, 10], the analytical expression

$$S(q, \gamma, \xi) = \frac{1}{[1/S_0(q, \xi)^2 + 4N^2\gamma[1 - G(\gamma, \xi)]/q^2]^{1/2}}.$$
(3)

 $S_0(q,\xi)$ is the SSF of the one-dimensional free-electron gas and is given by

$$S_0(q,\xi) = (1+\xi)S_{0+}(q)/2 + (1-\xi)S_{0-}(q)/2$$

with

$$S_{0\pm}(|q| \le 2k_{F\pm}) = |q|/2k_{F\pm}$$
 and $S_{0\pm}(|q| \ge 2k_{F\pm}) = 1$.

The factor containing $\gamma[1 - G(\gamma)]$ represents the contribution of the collective modes to the SSF. In the following, equation (2) and equation (3) are solved numerically.



Figure 1. The local-field correction $G(\gamma, \xi)$ versus the interaction strength parameter γ for different values of the spin-polarization parameter ξ calculated within the STLS approach. The scale on the r.h.s. shows the pair distribution function $g(z = 0) = 1 - G(\gamma, \xi)$.

Within the Hartree–Fock approximation (HFA), where $S(q, \gamma, \xi)$ is replaced by $S_0(q, \xi)$, one gets

$$G_{HFA}(\gamma,\xi) = (1+\xi^2)/2.$$
 (4)

This form of the LFC determines the compressibility and the spin susceptibility within the HFA. Note that $G_{HFA}(\gamma, \xi = \pm 1) = 1$. For the fully polarized electron gas one finds [11]

$$G(\gamma, \xi = \pm 1) = 1 \tag{5}$$

and the system is non-interacting: $X(q, \omega) = X_0(q, \omega)$. This is the exact result [12]. Numerical results for $G(\gamma, \xi)$ versus γ and versus ξ are shown in figure 1 and figure 2, respectively. Note, that $G(\gamma, \xi \to 0) \propto \xi^2$; see figure 2. The pair-correlation function g(z) within the STLS approach is expressed as $g(z = 0) = 1 - G(\gamma, \xi)$ and g(z = 0) is shown on the r.h.s. in figure 1 and in figure 2. $G(\gamma, \xi = 0)$ was discussed in reference [7].

3. Ground-state energy

The GSE $\varepsilon_g(\gamma, \xi)$ per particle defines the total energy (per length) $E_g(\gamma, \xi) = N\varepsilon_g(\gamma, \xi)$. In the following we use the notation $\varepsilon_g(\gamma, \xi) = N^2 \varepsilon_0(\gamma, \xi)/2m$ and give explicit expressions for $\varepsilon_0(\gamma, \xi)$, which is a dimensionless function of γ and ξ . The LFC determines the GSE via

$$\varepsilon_0(\gamma,\xi) = \frac{\pi^2}{12}(1+3\xi^2) + \int_0^{\gamma} d\lambda \ [1 - G(\lambda,\xi)].$$
(6)



Figure 2. The local-field correction $G(\gamma, \xi)$ versus the spin-polarization parameter ξ (plotted versus ξ^2) for different values of the interaction strength parameter γ calculated within the STLS approach. The dotted line represents the HFA. The scale on the r.h.s. shows the pair distribution function $g(z = 0) = 1 - G(\gamma, \xi)$.

The ground-state energy can also be written as [13]

$$\varepsilon_0(\gamma,\xi) = \varepsilon_{kin}(\xi) + \varepsilon_{HFA}(\gamma,\xi) + \varepsilon_{cor}(\gamma,\xi)$$
(7)

with the kinetic (kin) energy contribution

$$\varepsilon_{kin}(\xi) = \pi^2 (1 + 3\xi^2) / 12 \tag{8a}$$

and the Hartree-Fock (HFA) energy contribution

$$\varepsilon_{HFA}(\gamma,\xi) = \gamma(1-\xi^2)/2. \tag{8b}$$

Note that the HFA is obtained by using $G_{HFA}(\gamma, \xi) = (1 + \xi^2)/2$. The correlation (cor) energy $\varepsilon_{cor}(\gamma, \xi)$ is given by

$$\varepsilon_{cor}(\gamma,\xi) = \int_0^{\gamma} d\lambda \ [G_{HFA}(\lambda,\xi) - G(\lambda,\xi)]. \tag{8c}$$

With

$$G(\lambda, \xi = \pm 1) = G_{HFA}(\lambda, \xi = \pm 1) = 1$$

we get

$$\varepsilon_{cor}(\gamma, \xi = \pm 1) = 0$$
 and $\varepsilon_0(\gamma, \xi = \pm 1) = \pi^2/3$

which is the exact result. In fact, due to the Pauli principle, electrons with parallel spins cannot interact via a short-range potential and the GSE of a fully polarized electron gas only contains the kinetic energy. That is why in the one-dimensional electron gas with a short-range interaction potential, the GSE is bounded by $\pi^2/12 \leq \varepsilon_0(\gamma, \xi) \leq \pi^2/3$. In general one finds $G(\lambda, \xi) > G_{HFA}(\lambda, \xi)$ —see figure 2—and the correlation energy is negative.

In reference [9] we calculated the GSE of our model within a ladder approximation and obtained the correct weak- and strong-coupling GSE. We found an analytical expression for the GSE as a function of the coupling parameter γ and as a function of the spin-polarization parameter ξ . Correspondingly, we derived quasi-exact analytical expressions for the compressibility and the spin susceptibility.

The GSE obtained within the STLS approach versus γ is shown in figure 3 for different values of the spin polarization. Quasi-exact analytical results obtained in reference [9] are



Figure 3. The ground-state energy per particle $\varepsilon_0(\gamma, \xi)$ versus the interaction strength parameter γ for different values of the spin-polarization parameter ξ . The dashed lines represent the STLS approach and the solid lines represent quasi-exact analytical results [9].

also shown. For $\xi \neq \pm 1$ we find that the validity range of the STLS results is small: $\gamma < 2$. Most interesting in figure 3 is the fact that $\varepsilon_0(\gamma, \xi = 0)$, calculated within the STLS approach, crosses $\varepsilon_0(\gamma, \xi = \pm 1) = \pi^2/3$ at a certain $\gamma = \gamma_e = 10.2$, which implies a Bloch instability [14]: $\varepsilon_0(\gamma > \gamma_e, \xi = \pm 1) < \varepsilon_0(\gamma > \gamma_e, \xi = 0)$. Of course, this instability is an artifact of the STLS approach and does not occur within the exact theory. Within the HFA, for the GSE one finds the instability at $\gamma = \gamma_{HFA} = \pi^2/2 = 4.935$. This value of γ_{HFA} is used in the following to define the validity range of the STLS approach. For the GSE we conclude that the validity range of the STLS approach is $\gamma < 2 \approx 0.4\gamma_{HFA}$. In section 6 we discuss the artificial Bloch instability in detail.

4. Compressibility

The compressibility κ can be expressed in terms of the second derivative of the GSE via $\partial^2 E_g / \partial N^2 = \pi v_F \kappa_0 / 2\kappa$ with $\kappa_0 = 4m/\pi^2 N^3$ as the compressibility of the free-electron gas [13]. The derivative with respect to N can be expressed as the derivative with respect to γ , and one finds

$$\frac{\kappa_0}{\kappa} = 1 + \frac{2\gamma}{\pi^2} + \frac{12}{\pi^2} \varepsilon_{cor} - \frac{8\gamma}{\pi^2} \frac{\partial \varepsilon_{cor}}{\partial \gamma} + \frac{2\gamma^2}{\pi^2} \frac{\partial^2 \varepsilon_{cor}}{\partial \gamma^2}.$$
(9)

The HFA is given by $\kappa_0/\kappa_{HFA} = 1 + 2\gamma/\pi^2$. Within the exact theory the following limits apply to the compressibility [9]: $1 < \kappa_0/\kappa < 4$.

Our numerical results obtained within the STLS approach and quasi-exact results [9] for κ_0/κ versus γ are shown in figure 4. We conclude that the STLS approach gives a reasonably good value for the compressibility, compared with the quasi-exact result for $\gamma < 10 \approx 2\gamma_{HFA}$ (for the difference smaller than 10% between the two values). We mention that the validity range for the compressibility is much larger than that for the GSE.

5. Spin susceptibility

The spin susceptibility κ_s can be expressed in terms of the second derivative of the GSE as $\partial^2 E_g/N^2 \partial \xi^2 = \pi v_F \kappa_0/2\kappa_s$ [13]. We find

$$\frac{\kappa_0}{\kappa_s} = 1 - \frac{2\gamma}{\pi^2} + \frac{2}{\pi^2}\alpha \tag{10}$$



Figure 4. The inverse compressibility $1/\kappa$ (in units of the inverse compressibility of the freeelectron gas $1/\kappa_0$) versus the interaction strength parameter γ . The solid line represents quasiexact analytical results [9]. The results obtained according to the HFA and via the STLS approach are shown as the dotted and dashed lines, respectively.

and

$$\alpha = \lim_{\xi \to 0} [\partial^2 \varepsilon_{cor}(\gamma, \xi) / \partial \xi^2]$$

is called the spin stiffness. Within the HFA one finds that $\kappa_0/\kappa_{sHFA} = 1 - 2\gamma/\pi^2$ and $\kappa_0/\kappa_{sHFA} = 0$ for $\gamma = \gamma_{HFA}$, which corresponds to the Bloch instability within the HFA already found from GSE calculations.



Figure 5. The inverse spin susceptibility $1/\kappa_s$ (in units of the inverse spin susceptibility of the free-electron gas $1/\kappa_0$) versus $\Delta\xi$ as calculated using $\alpha = 2[\varepsilon_{cor}(\xi) - \varepsilon_{cor}(0)]/\Delta\xi^2$ and $\Delta\xi = \xi$ for an interaction strength parameter $\gamma = 5$.

We have calculated the spin stiffness from $\alpha = 2[\varepsilon_{cor}(\gamma, \xi) - \varepsilon_{cor}(\gamma, \xi = 0)]/\Delta\xi^2$ with $\Delta\xi = \xi$. Due to the fact that $G(\gamma, \xi)$, and correspondingly $\varepsilon_{cor}(\gamma, \xi)$, versus ξ^2 is not a straight line—see figure 2— α depends on $\Delta\xi$. This is seen in figure 5 where the inverse spin susceptibility versus $\Delta\xi$ for $\gamma = 5$ is shown. Of course, only the limit $\Delta\xi \rightarrow 0$ represents the true inverse spin susceptibility. In the literature we found calculations where the stiff stiffness for an electron gas with long-range Coulomb interaction is estimated from $\varepsilon_{cor}(\gamma, \xi = 1) - \varepsilon_{cor}(\gamma, \xi = 0)$, which corresponds to $\Delta\xi = 1$. We want to stress that this method, applied to the present model, gives results for the spin stiffness α depending on $\Delta\xi$.

The inverse spin susceptibility versus the interaction strength parameter γ is shown in figure 6. The quasi-exact spin susceptibility is given by $\kappa_0/\kappa_s = 1/[1 + 2\gamma/\pi^2]$ [9]: no



Figure 6. The inverse spin susceptibility $1/\kappa_s$ (in units of the inverse spin susceptibility of the free-electron gas $1/\kappa_0$) versus the interaction strength parameter γ . The solid line represents quasi-exact analytical results [9]. The dashed, dashed–dotted and dashed–double-dotted lines represent the STLS approach, where the spin stiffness is calculated with $\alpha = 2[\varepsilon_{cor}(\xi) - \varepsilon_{cor}(0)]/\Delta\xi^2$ and $\Delta\xi = \xi$. The HFA is shown as the dotted line. In the inset we show γ_c (defined by $\kappa_0/\kappa_s = 0$) versus $\Delta\xi$. The value obtained within the HFA ($\gamma_{HFA} = 4.9$) is indicated.

Bloch instability occurs. Due to the artificial Bloch instability within the STLS approach see figure 3—we find $\kappa_0/\kappa_s = 0$ at a critical parameter γ_c . γ_c versus $\Delta \xi$, used for the calculation of α , is shown in the inset of figure 6. Strictly speaking, the spin stiffness corresponds to the limit $\Delta \xi \rightarrow 0$, and the line with $\Delta \xi = 0.05$ in figure 6 represents the spin susceptibility within the STLS approach. For $\Delta \xi = 0.05$ one gets the Bloch instability at $\gamma_c \approx 22$. By comparing the STLS result with the quasi-exact result obtained in reference [9], we conclude that the STLS approach give reasonable results for the spin stiffness for $\gamma < 10 \approx 2\gamma_{HFA}$. The fact that we found $\gamma_c = 10.2 = \gamma_e$ for $\Delta \xi = 1$ can be easily understood from figure 3, where $\varepsilon_0(\gamma, \xi = 0) = \varepsilon_0(\gamma, \xi = 1)$ for $\gamma = \gamma_e$.



Figure 7. The spin stiffness α (shown as α/γ) versus the interaction strength parameter γ . The dotted line corresponds to the STLS approach derived from GSE calculations with $\Delta \xi = 0.05$. The solid line represents quasi-exact results [9].

In order to understand better the origin of the differences between the STLS approach and the quasi-exact result for κ_0/κ_s , we have plotted in figure 7 the ratio α/γ versus γ . We note the small differences between the quasi-exact result (where no Bloch instability occurs) and the STLS approach (with an artificial Bloch instability at $\gamma_c = 22$). This shows that the spin susceptibility is, in the strong-coupling limit, very sensitive to a correct calculation of the spin stiffness. We have plotted α/γ in figure 7: α is a strongly varying function of γ . In fact, α has, for large γ , to compensate for the strongly negative part of the spin susceptibility obtained within the HFA. In any approximating theory one will encounter difficulties in attempting to represent this compensation correctly (such that $\kappa_0/\kappa_s > 0$).

6. Discussion

The aim of the present paper was to calculate the compressibility and the spin susceptibility from GSE calculations and to determine the validity range of the STLS approach.

From the GSE calculation within the STLS approach we conclude that the polarized state is stable ($\varepsilon_0(\gamma, \xi = \pm 1) < \varepsilon_0(\gamma, \xi = 0)$) for $\gamma > 10.2$; see figure 3. Therefore, one could conclude that a Bloch instability occurs for $\gamma_e = 10.2$ (*e* standing for energy) and that for $\gamma \ge \gamma_e$ our calculations do not make any sense any longer. Of course, this instability is an artifact of the STLS approach. However, for the compressibility and the spin susceptibility we get good agreement with quasi-exact results for $\gamma < 10$ —see figure 4 and figure 5—and no instability is found in the spin susceptibility for $\gamma < 22$. The conclusions that we draw from these observations are the following:

(i) the STLS results for the compressibility and the spin susceptibility can be trusted for $\gamma < 10 \approx 2\gamma_{HFA} \approx \gamma_e$;

(ii) the validity range of GSE calculations within the STLS approach is smaller: $\gamma < 0.4 \gamma_{HFA} \approx 0.2 \gamma_e$; and

(iii) one can get artificial instabilities within the STLS approach.

The result concerning an artificial Bloch instability within the STLS approach is of some importance: for a long-range Coulomb interaction it was claimed recently that a Bloch instability could occur in quasi-one-dimensional systems [15]. This claim contradicts the theorem of Lieb and Mattis [16] which indicates that a polarized one-dimensional electron gas always has a larger GSE as an unpolarized electron gas. From the present paper we learned that the STLS approach *can* lead to an artificial Bloch instability at $\gamma_e = 10.2$ if one uses the GSE (and at $\gamma_c = 22$ if one uses the spin susceptibility). However, for $\gamma < 2\gamma_{HFA} \approx \gamma_e$ the STLS results obtained for the compressibility and the spin susceptibility can be trusted.

In the case of a long-range Coulomb interaction potential, the instability derived from the GSE (*e* standing for energy) occurred at $r_s \ge r_{se} \approx 1.4r_{seHFA} \approx 1-4$, depending on the wire width [15]. $r_s = 1/2Na^*$ is the Wigner–Seitz parameter with a^* as the effective Bohr radius. The factor 1.4 indicates that correlation effects are not yet very important and that the instability is dominated by exchange effects. Therefore, we believe that the instability for the long-range Coulomb interaction [8, 15] *might* be a real effect. Experimental evidence for this instability was cited in reference [8]. But we admit that more experiments are needed. However, independently of the existence (or non-existence) of this instability, we conclude from the results obtained in the present paper that the numerical values for the spin susceptibility obtained in reference [8] are expected to be correct for $r_s < r_{se}$.

Using a ladder approach it was argued that a Bloch instability occurs for $\gamma_e = 23.6$ [17]. This artificial instability again has its origin in the wrong strong-coupling limit of the ground-state energy found in reference [17]: $\varepsilon_0(\gamma \to \infty, \xi = 0) = 1.21\pi^2/3$ instead of the exact result $\varepsilon_0(\gamma \to \infty, \xi = 0) = \pi^2/3$. This shows that the prediction of a Bloch instability is a non-trivial problem if exact results for the GSE are not available. In our analytical approach within a simplified ladder theory, we obtained $\pi^2/12 \leq \varepsilon_0(\gamma, \xi) \leq \pi^2/3$

and no Bloch instability was found [9].

We believe that a short-range interaction potential is the most unfavourable potential for the application of the STLS approach: the GSE within the STLS approach becomes completely wrong for large coupling: $\varepsilon_0(\gamma \to \infty, \xi = 0) \propto \ln(\gamma)$ [6, 7] while the exact result is $\varepsilon_0(\gamma \to \infty, \xi) = \pi^2/3 = 3.29$. This is not the case if the STLS approach is used for systems with a long-range interaction potential [11, 18]. Therefore, we believe that the STLS results for the compressibility [18] and the spin susceptibility [8] of quasione-dimensional systems with a long-range interaction potential can be trusted at least up to $r_s < r_{se}$. A more conservative estimate would be $r_s < r_{seHFA}$.

7. Conclusion

We have presented results for the ground-state energy, the compressibility and the spin susceptibility of a one-dimensional electron gas with a short-range interaction potential obtained by using a *generalized* STLS approach. From comparing with quasi-exact results we conclude that the STLS approach gives quantitatively correct results for the compressibility and the spin susceptibility if $\gamma < 10 \approx 2\gamma_{HFA}$. The results obtained for the ground-state energy are found to be less correct and the validity range is estimated as $\gamma < 2 \approx 0.4\gamma_{HFA}$.

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