Short-range correlations in a one-dimensional electron gas

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We use the Singwi-Sjölander-Tosi-Land (SSTL) approximation to investigate the short-range correlations in a one-dimensional electron gas. We find out that the SSTL approximation satisfies the compressibility sum rule somewhat better than the more widely used Singwi-Tosi-Land-Sjölander approximation in the case of a one-dimensional electron gas.

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I. INTRODUCTION

Recent technological advances in fabrication technologies have made it possible to produce effectively one-dimensional (1D) semiconductor structures or quantum wires.[1–5] These progresses, indeed, have made the 1D electronic systems one of the most attractive subjects of both theoretical and experimental condensed matter physics for some decays. It is well known that quantum confinement increases the role played by many-body effects due to the severe restrictions in the phase space as in 1D electronic systems. Naturally, there are numerous theoretical investigations dedicated to understanding these effects.[6–13]

The exchange and correlation effects describing the screening properties of a system of electrons interacting via the long-range Coulomb interaction potential at high densities is well explained by a mean-field approach: the random-phase approximation (RPA). However, as the particle density is lowered exchange-correlation effects become important and the RPA fails to explain the physical properties of the system. The Singwi-Tosi-Land-Sjölander[14] (STLS) has been introduced as an improvement over the RPA to take into account short-range correlation effects in terms of a local field correction (LFC) which considers the repulsion hole around an electron.

Extensive investigations of three-dimensional electron gas have clearly shown the importance of short-range correlations at lower densities in determining the pair distribution function $g(\mathbf{r})$ at small $\mathbf{r}$.[15] Although the STLS approximation gives a correct pair correlation function and ground-state energy, it fails to satisfy the compressibility sum rule. In order to satisfy the compressibility sum rule, there have been several attempts.[16,17] In the Singwi-Sjölander-Land-Tosi (SSTL) approximation, the interaction potential entering the LFC expression is screened by the static dielectric function in order to include the effect of screening on the effective potential.

In this work, our main motivation is to inquire the performance of both SSTL and STLS approaches in a 1D electron gas as far as the compressibility is concerned. To the best of our knowledge, this is the first application of the SSTL approach in lower dimensions.

The outline of this paper is as follows. The quantum wire model we assume in this work and the STLS and SSTL formalisms are given in Sec. II. The results and a discussion concentrating on a comparison between STLS and SSTL performances in the compressibility issue are presented in Sec. III.

II. MODEL AND THEORY

Currently fabricated semiconductor quantum wires are long 1D structures with a finite lateral width. We assume that electrons are constrained to move only in one direction by a harmonic confinement. Such a model yields the Coulomb interaction between the electrons $V(q)=(e^2/\epsilon_0)\times\exp(b^2q^2/4)K_0(b^2q^2/4)$, where $K_0(x)$ is the modified Bessel function of the second kind. The parameter b is related to the confining potential, and it is a measure of the effective diameter of the quantum wire.[18] The linear number density n is defined in terms of the spin and valley degeneracies g_s and g_ν, respectively, and the Fermi wave number k_F as $n=g_sg_\nu k_F/\pi$. In this paper, we use $g_\nu=1$. The dimensionless density parameter r_s is related to the linear density as $r_s=1/(2na_B^\star)$, where $a_B^\star=\epsilon_0/(e^2m^\star)$ is the effective Bohr radius in the semiconducting wire with background dielectric constant ϵ_0 and electron effective mass $m^\star$ (we take $\hbar=1$). In this work, we employ the single-subband approximation, which implies that the intersubband energy distance is larger than the Fermi energy. In other words, electrons occupy only the first subband, which requires that $r_s>(\pi/2^{5/2})(b/a_B^\star)$.[7]

A. Self-consistent equations

The quantity having central importance in characterizing a many-body system is the wave-vector- and frequency-dependent density-density response function $\chi(q,\omega)$. In the STLS theory, this function is given in terms of the LFC $G(q)$ as

$$\chi(q,\omega)=\frac{\chi_0(q,\omega)}{1-V(q)[1-G(q)]\chi_0(q,\omega)}, \tag{1}$$

where $\chi_0(q,\omega)$ is the zero-temperature susceptibility of the noninteracting electron gas and it is given by

$$\chi_0(q,\omega)=\frac{m^\star}{\pi q}\ln\left|\frac{\omega^2-\omega_-^2}{\omega^2-\omega_+^2}\right|, \tag{2}$$

where $\omega_\pm=|q^2/2m^\star\pm 2qk_F/m^\star|$ are the boundaries of the

particle-hole continuum. The static structure factor is related to the density-density response function through the fluctuation-dissipation theorem as

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

where we perform frequency integration along the imaginary axis by using Wick rotation. The static LFC arising from the exchange-correlation effects and short-range Coulomb correlations is given by

$$G(q) = -\frac{1}{n}\int_{-\infty}^{\infty}\frac{dq'}{2\pi}\frac{q'}{q}\frac{V(q')}{V(q)}[S(q-q')-1]. \tag{4}$$

The set of equations (1), (3), and (4) has to be solved self-consistently for $\chi(q)$, $S(q)$, and $G(q)$ within the STLS approximation. In the RPA, $G(q)=0$.

The SSTL approximation is different from the STLS approximation in that the interaction potential is screened by the static dielectric function, which is expressed in the form

$$\epsilon(q) = 1 - \frac{V(q)\chi_0(q)}{1+G(q)V(q)\chi_0(q)}. \tag{5}$$

This is originally done to better satisfy the compressibility sum rule in three-dimensional electron gas.

Finally, the pair correlation function can be calculated by the Fourier transform of the static structure factor as

$$g(r) = 1 + \frac{1}{2}\int_0^\infty dq \cos(qr)[S(q)-1]. \tag{6}$$

A. Ground-state energy and compressibility

The calculation of the ground-state energy is an easy task once the dielectric function is determined. The ground-state energy per particle, ε_g, can be defined in terms of kinetic, exchange, and correlation contributions as

$$\varepsilon_g(r_s) = \varepsilon_{kin}(r_s) + \varepsilon_{exc}(r_s) + \varepsilon_c(r_s). \tag{7}$$

The $\varepsilon_g(r_s)$ for a 1D electron system may be expressed as

$$\varepsilon_g(r_s) = \varepsilon_{kin}(r_s) + \frac{1}{4r_s}\int_0^1 d\lambda \int_0^\infty dq F(q)[S(q,\lambda)-1], \tag{8}$$

where λ is the coupling constant and $F(q)=V(q)/(e^2/\epsilon_0)$. The kinetic energy per particle of a 1D electron gas is given as $\varepsilon_{kin}(r_s)=\pi^2/48r_s^2$.

The exchange energy per particle is given by

$$\varepsilon_{exc}(r_s) = \frac{1}{4r_s}\int_0^2 dq F(q)[q/2-1]. \tag{9}$$

All the energies above are in effective Rydberg units [$\mathrm{Ry}^\star = 1/(2m^\star a_B^{\star 2})$].

The correlation energy is the difference between the Hartree-Fock ground-state energy and any better calculation. It can be computed via Eq. (7), if we know other terms.

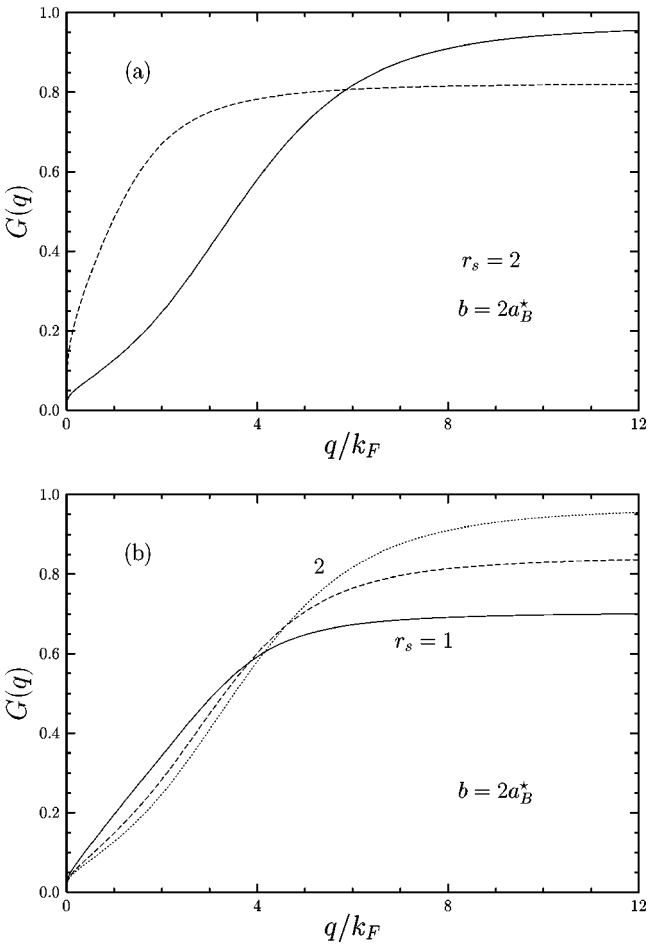

FIG. 1. The local field correction $G(q)$ for a quantum wire of width $b=2a_B^\star$. (a) Comparison of the SSTL (solid line) and STLS (dashed line) approximations at $r_s=2$. (b) The SSTL performance at $r_s=1$, 1.5, and 2.

The isothermal compressibility κ is an important macroscopic property of the system. It can be computed either by using the second derivative of the ground-state energy per particle,

$$\frac{\kappa_0}{\kappa} = \frac{8r_s^4}{\pi^2}\frac{d^2\varepsilon_g}{dr_s^2}, \tag{10}$$

or by using the long-wavelength limit of the static dielectric function of the electron gas system, $\lim_{q\to 0}\epsilon(q)=1+V(q)n^2\kappa$, which yields

$$\frac{\kappa_0}{\kappa} = 1 + \frac{4r_s}{\pi^2}\int_0^\infty dq F(q)\ln\left|\frac{2-q}{2+q}\right|\frac{dS(q)}{dq}, \tag{11}$$

where $\kappa_0 = 32m^\star r_s^3 a_B^{\star 3}/\pi^2$ is the free-electron gas compressibility. We note that in Eqs. (8), (9), and (11), the wave number q is normalized by k_F.

The compressibility sum rule requires the compressibility computed in the two different methods to be the same.

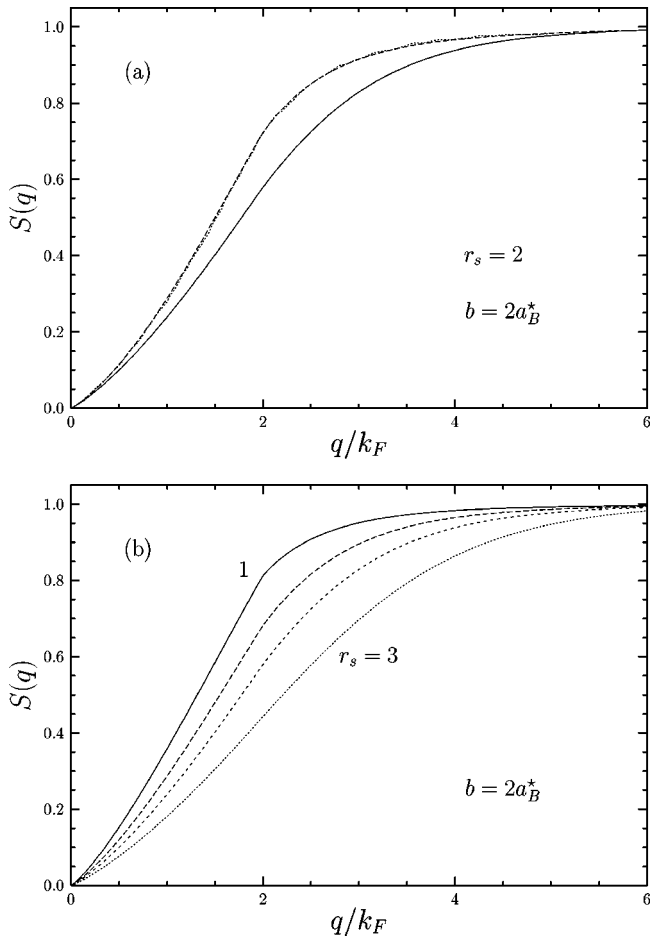

FIG. 2. The static structure factor $S(q)$ for a quantum wire of width $b=2a_B^\star$. (a) Comparison of the SSTL (solid line) and STLS (dashed line) approximations at $r_s=2$. The dotted line is the result of Tanatar (Ref. 19) which cannot be resolved since the results are almost identical. (b) The SSTL performance at $r_s=1$, 1.5, 2, and 3.

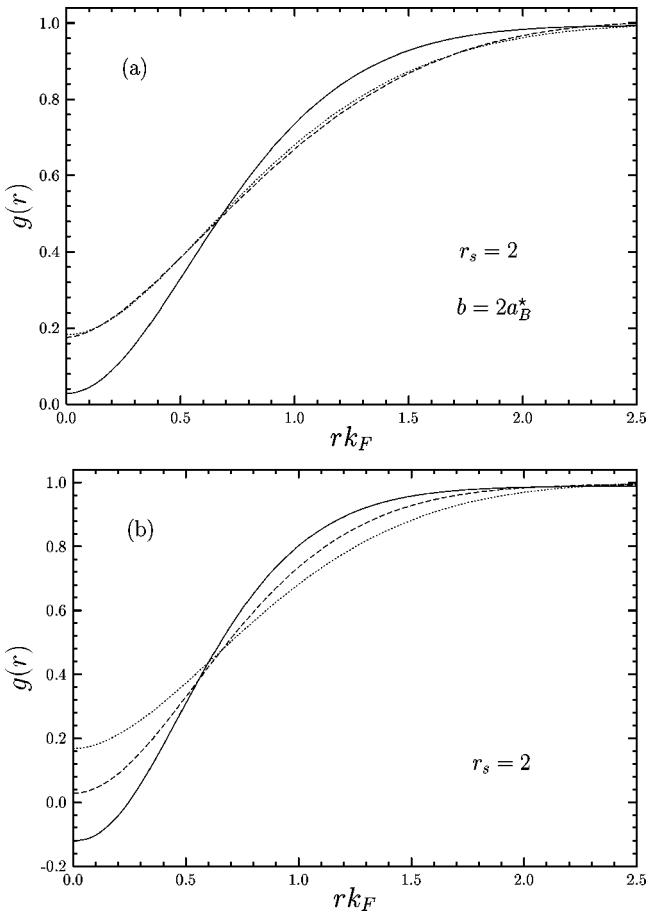

FIG. 3. The pair correlation function $g(r)$ (a) in the SSTL approximation (solid line), STLS approximation (dashed line), and Ref. 19 (dotted line) at $r_s=2$ and $b=2a_B^\star$. (b) SSTL performance at $r_s=2$ for quantum wire widths of $b=a_B^\star$ (solid line), $b=2a_B^\star$ (dashed line), and $b=4a_B^\star$ (dotted line).

III. RESULTS AND DISCUSSION

We solve the set of equations [Eqs. (1), (3), and (4)] that describes the density response, static structure factor, and the local field correction self-consistently. The numerical accuracy attained in the calculations is 0.001%.

In Fig. 1(a) we compare the local field correction $G(q)$ calculated in the SSTL and STLS approximations for the same wire radius and electron density. The most striking difference between the curves is their large-q limits. The STLS curve increases faster with q and saturates at relatively small q while SSTL $G(q)$ saturates at a larger q value. We also observe that $G(q\rightarrow\infty)$ in the SSTL approximation is larger than that in the STLS approximation. On the other hand, $G(q\rightarrow 0)\propto 1/V(q\rightarrow 0)$ in both approximations as expected. The SSTL $G(q)$ behavior at different densities is displayed in Fig. 1(b). We point out that with decreasing density (equivalently with increasing r_s), the $G(q)$ increases, which means that the correlations between electrons are getting important.

The static structure factor $S(q)$ in different approximations for $r_s=2$ is shown in Fig. 2(a). The curves obtained in both SSTL and STLS approximations are similar. Moreover, we observe that our STLS result is in good agreement with that of Tanatar[19] at the same density. In Fig. 2(b) we plot $S(q)$ within the SSTL approximation for $r_s=1$, 1.5, 2, and 3. Notice that the large-q limit of $S(q)$ is correctly given as

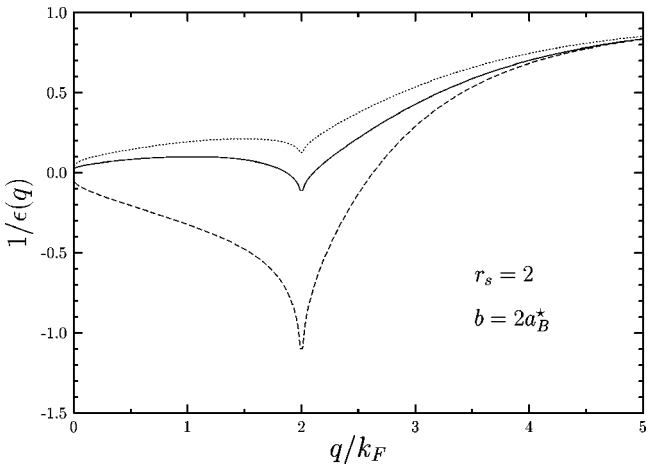

FIG. 4. The inverse dielectric function in the SSTL approximation (solid line), STLS approximation (dashed line), and RPA (dotted line) at $r_s=2$ and $b=2a_B^\star$.

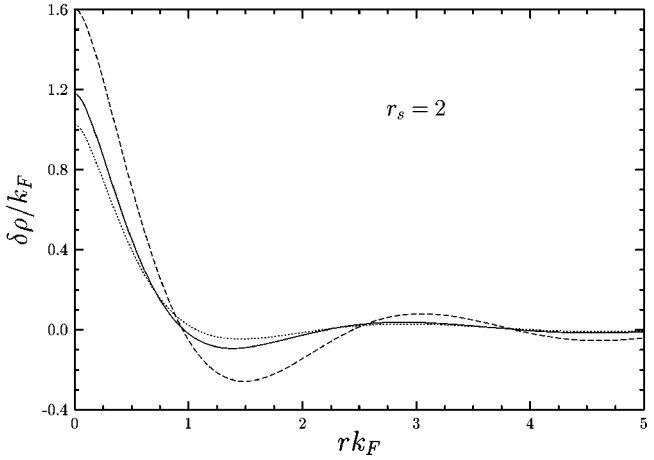

FIG. 5. The screening charge density near a point impurity in the 1D electron gas with $r_s=2$ calculated in the SSTL approximation (solid line), STLS approximation (dashed line), and RPA (dotted line) for $b=2a_B^\star$.

1. As the density is lowered, $S(q)$ value is getting smaller as expected.

The probability of finding an electron at r if another electron is located at the origin is given by the pair correlation function $g(r)$. We notice that for the same density, a small r value of $g(0)$ is positive in both the STLS and SSTL approximations. Moreover, the STLS $g(0)$ is greater than the SSTL value as is seen in Fig. 3(a). Again we observe a very good agreement between the STLS results of the present work and Ref. 19. The behavior of $g(r)$ in the SSTL approximation for $b/a_B^\star=1$, 2, and 4, but at the same density, is shown in Fig. 3(b). We find that $g(0)$ gets larger as b increases and $g(0)$ is negative for $b=a_B^\star$. The one-dimensional interaction potential $V(q)$ is weakened as b increases. Investigation of $g(r)$ as a function of r_s showed that $g(0)$ becomes negative for $r_s>5.1$ in the STLS approximation, and $r_s>2.1$ in the SSTL approximation when $b=2a_B^\star$. Our findings for STLS $g(0)$ are in good agreement with the results of Ref. 7.

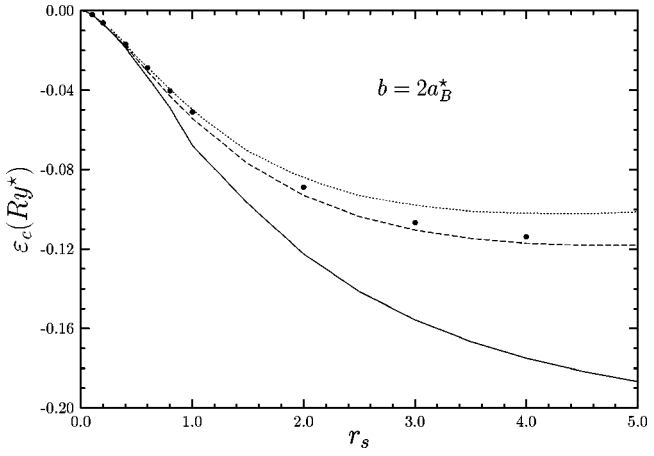

FIG. 6. The correlation energy per particle as a function of r_s in the SSTL (solid line) and STLS (dashed line) approximations for $b=2a_B^\star$. The dotted line shows the results of Ref. 21, and the solid circles show those of Ref. 7.

TABLE I. Correlation energies $\varepsilon_{cor}(r_s,b)$ per particle (in units of the effective Rydberg Ry*) for $b=a_B^\star$, $b=2a_B^\star$, and $b=4a_B^\star$ obtained within the SSTL approximation.

r_s	$-\varepsilon_{cor}(r_s,b=a_B^\star)$	$-\varepsilon_{cor}(r_s,b=2a_B^\star)$	$-\varepsilon_{cor}(r_s,b=4a_B^\star)$
0.1	0.006 731	0.002 100	0.000 633
0.2	0.019 901	0.006 502	0.002 033
0.4	0.054 148	0.018 774	0.006 145
0.6	0.091 337	0.033 444	0.011 328
0.8	0.126 239	0.048 900	0.017 139
1.0	0.156 726	0.067 816	0.023 271
2.0	0.249 965	0.122 460	0.052 289
3.0	0.289 631	0.155 645	0.073 565
4.0	0.306 768	0.174 948	0.088 268
5.0	0.313 627	0.186 701	0.098 608

The inverse dielectric function in the SSTL approximation is plotted in Fig. 4. This is rather similar to the RPA result whereas the STLS $1/\epsilon(q)$ is more pronounced. All curves

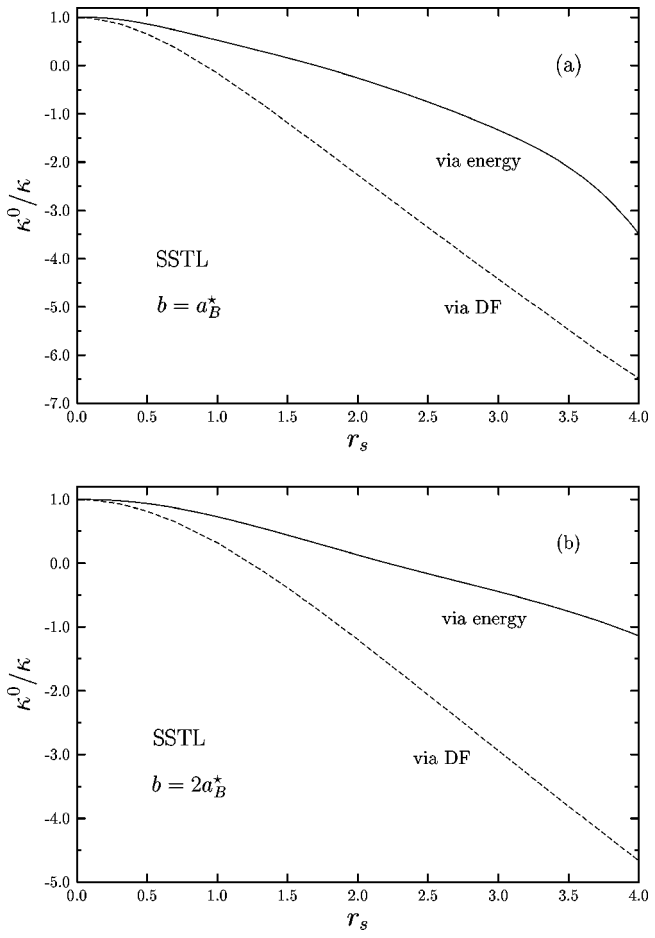

FIG. 7. Normalized inverse compressibility by using the ground-state energy per particle and dielectric function in the SSTL approximation for a quantum wire of width (a) $b=a_B^\star$ and (b) $b=2a_B^\star$.

have a discontinuity in the derivative at $q=2k_F$.

The density of screening charge $\delta\rho$ at a distance r from a static point impurity of unit charge located at the center of the wire is given by the relation[20]

$$\delta\rho(r)=\int \frac{dq}{2\pi}e^{iqr}\left[\frac{1}{\epsilon(q)}-1\right]. \tag{12}$$

The $\delta\rho$ calculated at $b=2a_B^\star$ and $r_s=2$ is given in Fig. 5. The SSTL and RPA curves are shallow and similar as a result of the $1/\epsilon(q)$ behavior whereas STLS curve shows a deeper minimum. The screening charge density has the Friedel oscillations at large distance as in the 3D case.[16]

The correlation energy is one of the main properties of the system. We present our ε_{cor} results for the SSTL and STLS approaches in Fig. 6. It is seen that the STLS approximation leads to a larger value for the correlation energy compared to the SSTL approximation. The difference between ε_{cor} results of the two models increases with increasing r_s. We find out that our results for the STLS approximation are very close to those of Gold and Calmels[7] and Tanatar and Bulutay[21] who used the same quantum model as we employ. The small difference should be attributed to the methods used in the calculations; the three-sum-rule approach for the local field correction is used in Ref. 7, whereas in Ref. 21, Rice's approach[22] is used for the correlation energy calculation. In Table I, we give some numerical results for the correlation energy for different b and r_s within the SSTL approximation.

The compressibility sum-rule calculation is the main aim of the present work. We investigate the compressibility sum rule in the SSTL approximation for wire widths $b=a_B^\star$ and $b=2a_B^\star$. The results are plotted in Fig. 7. The inverse normalized compressibility computed via both the energy and dielectric functions is larger (in magnitude) in the same density range for the wire with smaller b, where the interaction potential is stronger. In Fig. 8, we compare our STLS compressibility results with those of Refs. 7 and 21. The results are in very good agreement. We notice that for the same wire width, $b=2a_B^\star$, the difference between the compressibility computed by using the ground-state energy per particle and the long-wavelength limit of the dielectric function is smaller in the SSTL approximation.

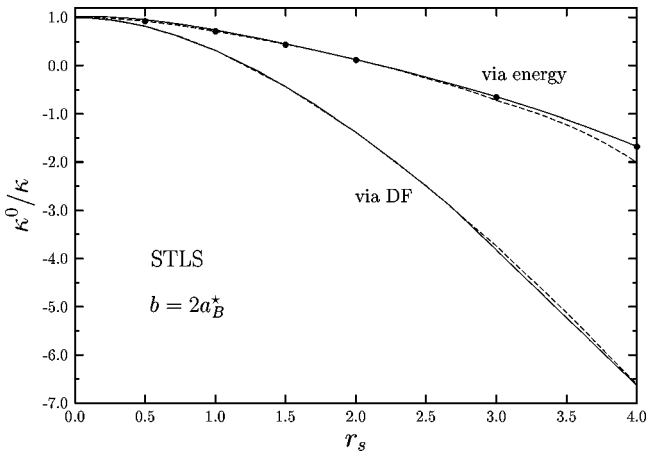

FIG. 8. Compressibility based on the ground-state energy per particle and dielectric function in the STLS approximation (solid line) and Ref. 21 (dashed line) for $b=2a_B^\star$. The solid circles are the results of Ref. 7 computed only via the ground-state energy.

In summary, we have studied the short-range correlations in a one-dimensional electron gas by using the SSTL approximation. The performance of the SSTL approximation is compared with the more widely used STLS approximation. We conclude that the SSTL approximation compares well with the STLS approximation when the static structure factor, pair correlation function, and dielectric function are considered. The most important finding of this work is that the SSTL approximation satisfies the compressibility sum rule somewhat better than the STLS approximation.

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