

Short range correlations in a one dimensional electron gas

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Abstract

We use the SSTL (Singwi, Sjölander, Tosi, Land) approximation to investigate the short-range correlations in a one dimensional electron gas, for the first time. Although SSTL is introduced to better satisfy the compressibility sum rule in three dimensions, the widely used STLS (Singwi, Tosi, Land, Sjölander) approximation turns out to be more successful in the case of the one dimensional electron gas.

Keywords: Quantum wires; Screening; Compressibility

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1 Introduction

The advances in fabrication technologies have made it possible to experimentally fabricate one dimensional electronic structures[1]–[5]. This has naturally resulted in an increasing interest in theoretical investigations of such structures[6]–[13]. The resulting one dimensional electron gas has also been subject to computational investigation[14].

The extensive investigations in the three dimensional electron gas have clearly shown the importance of the short range correlations at lower densities in determining the pair distribution function $g(r)$ at small r [15].

In the high density limit, the long range correlations can be described well by the random phase approximation (RPA). One way to include the short range correlation effects beyond RPA is to use the powerful approach developed by STLS[16].

It is well known that STLS approach suffers from a compressibility inconsistency. The compressibility calculated from the small q limit of the dielectric function $\varepsilon(q)$ does not agree with that calculated from the ground state energy. There have been several attempts to overcome this inconsistency[17, 18]. SSTL[17] included the effect of screening on the effective interaction potential as explained in the next section.

In this work, we aim to check the performance of the SSTL approach and compare it with the STLS in a one dimensional electron gas. To the best of our knowledge, this is the first application of the SSTL approach in lower dimensions.

The organization of the paper is as follows; the STLS and SSTL formalisms are given in section 2. The results and discussion concentrating on the comparison between STLS and SSTL performance on the compressibility issue are presented in section 3.

2 Formalism

In the mean field approximation, a key component of the electron gas is the usual static structure factor $S(q)$ which is related to density–density response function $\chi(q, \omega)$ through the fluctuation–dissipation theorem as

$$S(q) = -\frac{1}{n\pi} \int_0^\infty d\omega \text{Im}\chi(q, \omega). \quad (1)$$

The density–density response function $\chi(q, \omega)$ is defined as

$$\chi(q, \omega) = \frac{\chi_0(q, \omega)}{1 - V_{eff}(q)\chi_0(q, \omega)}, \quad (2)$$

where $\chi_0(q, \omega)$ is the zero–temperature susceptibility of a noninteracting electron gas and is given in one dimension by

$$\chi_0(q, \omega) = \chi_{01}(q, \omega) + i\chi_{02}(q, \omega), \quad (3)$$

with

$$\chi_{01}(q, \omega) = \frac{m^*}{\hbar^2 \pi q} \ln \left| \frac{\omega^2 - \omega_-^2}{\omega^2 - \omega_+^2} \right|, \quad (4)$$

and

$$\chi_{02}(q, \omega) = \begin{cases} -\frac{m^*}{\hbar^2 q}, & \omega_- < \omega < \omega_+ \\ 0 & \text{otherwise,} \end{cases}$$

where $\omega_{\pm} = \left| \frac{\hbar^2 q^2}{2m^*} \pm \frac{\hbar q k_F}{m^*} \right|$ are the boundaries for particle-hole excitations. The Fermi wave vector k_F is related to the one dimensional electron density n via $k_F = n\pi/2$. The dimensionless electron density parameter is defined as $r_s = \pi/(4k_F a_B^*)$, where a_B^* is the effective Bohr radius.

$V_{eff}(q)$ in Eq. (2) is the self-consistent effective potential related to the static structure factor through

$$V_{eff}(q) = v(q) + \frac{1}{nq} \int_0^{\infty} \frac{dk}{2\pi} [S(k) - 1] \{(q+k)v(q+k) + (q-k)v(q-k)\}, \quad (5)$$

where $v(q)$ is the Fourier transform of the Coulomb interaction between two electrons in the lowest subband in the harmonic confinement in one dimension and is given by

$$v(q) = \frac{2e^2}{\varepsilon_0} F(q), \quad (6)$$

where ε_0 is the background dielectric constant, q is the wave vector along the wire and $F(q)$ is the form factor which takes into account the finite thickness of the wire. The form factor reads

$$F(q) = \frac{1}{2} \exp\left(\frac{b^2 q^2}{4}\right) K_0\left(\frac{b^2 q^2}{4}\right), \quad (7)$$

here $K_0(x)$ is the zeroth order modified Bessel function of the second kind and b is the characteristic length of the harmonic potential. Indeed, it is a measure of the effective radius of the quantum wire[19].

In the STLS approximation,

$$\chi(q, \omega) = \frac{\chi_0(q, \omega)}{1 - v(q)[1 - G(q)]\chi_0(q, \omega)}, \quad (8)$$

where the local field correction $G(q)$ is

$$G(q) = -\frac{1}{n} \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{k}{q} \frac{v(k)}{v(q)} [S(q-k) - 1]. \quad (9)$$

The set of Eqs. (1), (8) and (9) have to be solved self-consistently for $G(q)$, $\chi(q)$ and $S(q)$ within the STLS approximation. In RPA, $G(q) = 0$.

The SSTL approximation is different from the STLS approximation in that the potential under the integral sign in Eq. (5) is screened by the static dielectric function $\varepsilon(q)$ which is given by,

$$\varepsilon(q) = 1 - \frac{v(q)\chi_0(q)}{1 + G(q)v(q)\chi_0(q)}. \quad (10)$$

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

The ground state energy per particle in one dimensional electron gas may be written as[20]

$$\varepsilon_g = \varepsilon_{kin} + \varepsilon_{ex} + \varepsilon_{cor}, \quad (11)$$

where ε_{kin} is the kinetic energy per particle, and simply $\varepsilon_{kin} = \pi^2/(48r_s^2)$ in units of effective Rydberg Ry^* . ε_{ex} is the exchange energy per particle

$$\varepsilon_{ex} = -\frac{1}{2\pi^2 n} \int_0^{k_F} dq \int_{-(k_F+q)}^{k_F-q} dk v(k), \quad (12)$$

and ε_{cor} is the correlation energy per particle

$$\varepsilon_{cor} = \frac{1}{2\pi r_s} \int_0^{r_s} dr'_s \int_0^\infty dq v(q) [S(q, r'_s) - 1]. \quad (13)$$

The compressibility K may be calculated either by using the ground state energy per particle ε_g

$$\frac{1}{K} = n^2 \frac{d^2}{dn^2} (n \varepsilon_g), \quad (14)$$

or by using the $q \rightarrow 0$ limit of the static dielectric function $\varepsilon(q)$

$$\lim_{q \rightarrow 0} \varepsilon(q) = 1 + v(q) n^2 K. \quad (15)$$

The compressibility sum rule is that the compressibilities calculated by using Eq. (14) and Eq. (15) are the same.

3 Results and Discussion

In Fig. 1 the local field correction $G(q)$ calculated self-consistently using STLS and SSTL approximations are shown for fixed $b = 5a_B^*$ and $r_s = 5$. The most striking difference between the two curves is their large q limits. As STLS $G(q)$ is approaching 1, SSTL $G(q)$ approaches a limit bigger than 1. It may be noted that the relation[18] $G(\infty) = 1 - g(0)$ is satisfied in our calculations. This, of course, is going to lead to different results when applied to physical properties of the one dimensional electron gas.

The different large q behaviour of $G(q)$ is expected to lead to different small r behaviour of the pair correlation function $g(r)$. This is shown in Fig. 2. As radius of the wire gets smaller the difference between STLS and SSTL results become larger, as may be seen in Fig. 3. As the density becomes smaller (i.e., r_s becomes larger) the SSTL $g(r)$ becomes negative for small r . This limit is where the correlation effects become important.

The SSTL $\varepsilon(q)^{-1}$ is given in Fig. 4. This is rather similar to STLS or RPA $\varepsilon(q)^{-1}$ with a discontinuity in the derivative at $q = 2k_F$.

The ground state energy per particle for our system is shown in Fig. 5. The STLS and SSTL curves are rather similar.

The compressibility calculated by using the ground state energy in three different approaches is presented in Fig. 6 as a function of r_s . The similarity in energies is also reflected in these curves. The negative compressibility values at higher r_s show that the system becomes unstable.

The compressibility calculated by using $q \rightarrow 0$ limit of the static dielectric function is shown in Fig. 7. Here, the STLS and SSTL compressibilities calculated by two routes are as different as in RPA. This surprising result is a natural consequence of the small q behaviour of the local field correction which is very small for SSTL at small q values.

The compressibility in a one dimensional system is studied previously by Gold and Calmels[7] using a three-sum-rule approach for the local field correction. The compressibility sum rule is better satisfied within this variant of STLS in one dimension as can be seen from their figure 4. We find the same result by the present full STLS calculation.

We can conclude that the short-range correlations are calculated using the SSTL approximation in a one dimensional electron gas, for the first time. The performance of the SSTL approximation is compared with the more widely used STLS approximation. It is shown that SSTL compares reasonably well with STLS when the pair correlation function, dielectric function and the ground state energy per particle are considered but fails totally when the compressibility sum rule is checked.

References

- [1] H. Temkin, G. J. Dolan, M. B. Panish, and S. N. G. Chu, Appl. Phys. Lett. **50**, 413 (1987).
- [2] J. H. F. Scott–Thomas, S. B. Field, M. A. Kastner, H. I. Smith, and D. A. Antoniadis, Phys. Rev. Lett. **62**, 583 (1989).
- [3] A. S. Plaut, H. Lage, P. Grambow, D. Heitmann, K. von Klitzing, and K. Ploog, Phys. Rev. Lett. **67**, 1642 (1991).
- [4] A. R. Goñi, A. Pinczuk, J. S. Wiener, J. M. Calleja, B. S. Dennis, L. N. Pfeiffer, and K. W. West, Phys. Rev. Lett. **67**, 3298 (1991).
- [5] M. S. Miller, H. Weman, C. E. Pryor, M. Krishnamurthy, P. M. Petroff, H. Kroemer, and J. L. Merz, Phys. Rev. Lett. **68**, 3464 (1992).
- [6] L. Calmes and A. Gold, Phys. Rev. B **52**, 10841 (1995).
- [7] A. Gold and L. Calmes, Solid State Commun. **100**, 137 (1996).
- [8] R. Fantoni, M. P. Tosi, Physica B **217**, 35 (1996).
- [9] S. Das Sarma and E. H. Hwang, Phys. Rev. B **54**, 1936 (1996).
- [10] A. Gold and L. Calmes, Phys. Rev. B **58**, 3497 (1998).
- [11] E. Demirel, B. Tanatar, Eur. Phys. J. B **12**, 47 (1999).
- [12] D. Schemerek, W. Hansen, Phys. Rev. B **60**, 4485 (1999).
- [13] B. Tanatar, E. Demirel, Phys. Status Solidi B **220**, 909 (2000).
- [14] A. Malatesta and G. Senatore, J. Phys IV **10**, 341 (2000).
- [15] K. S. Singwi and M. P. Tosi, in *Solid State Physics*, edited by F. Seitz, H. Ehrenreich, and D. Turnbull (Academic, New York, 1981), vol. 36, p. 177.
- [16] K. S. Singwi, M. P. Tosi, R. H. Land and A. Sjölander, Phys. Rev. **176**, 589 (1968).
- [17] K. S. Singwi, A. Sjölander, M. P. Tosi and R. H. Land, Phys. Rev. **1**, 1044 (1970).
- [18] P. Vashista and K. S. Singwi, Phys. Rev. B **6**, 875 (1972).
- [19] G. Y. Hu and R. F. O’Connell, Phys. Rev. B **42**, 1290 (1990).
- [20] V. B. Campos, M. H. Degani and O. Hipolito, Superlattice Microstructures **17**, 85 (1995).

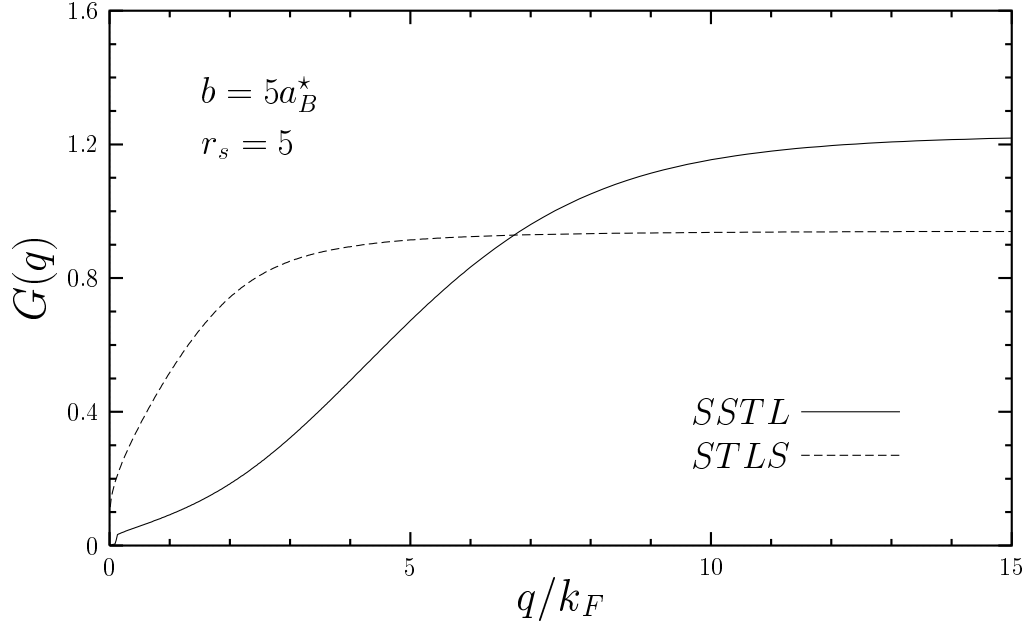


Figure 1: The local field correction in SSTL and STLS approximations for wire radius $b = 5a_B^*$ and $r_s = 5$.

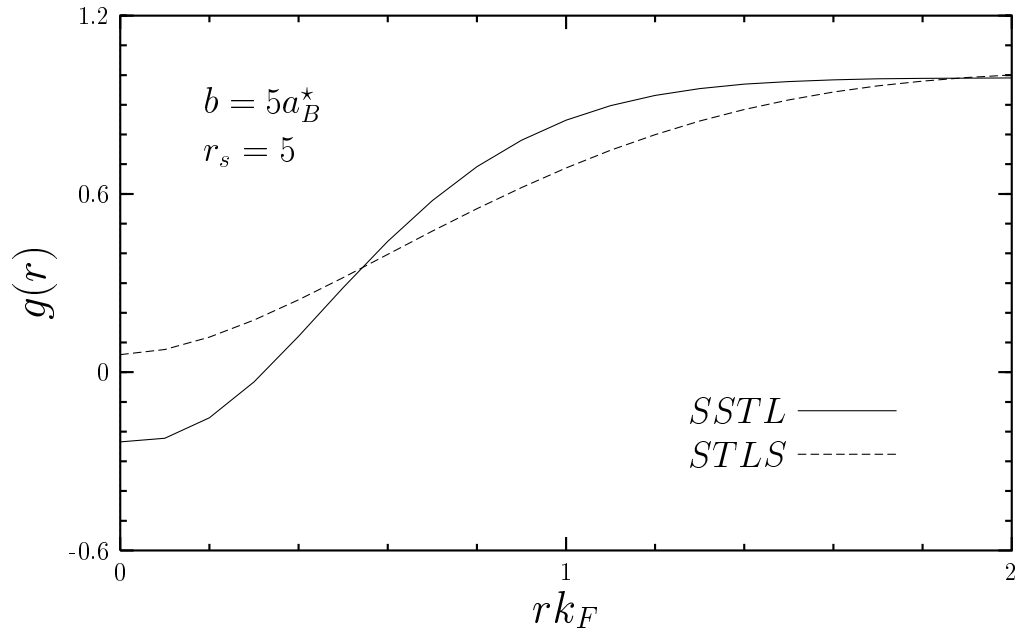


Figure 2: The pair correlation function in SSTL and STLS approximations for wire radius $b = 5a_B^*$ and $r_s = 5$.

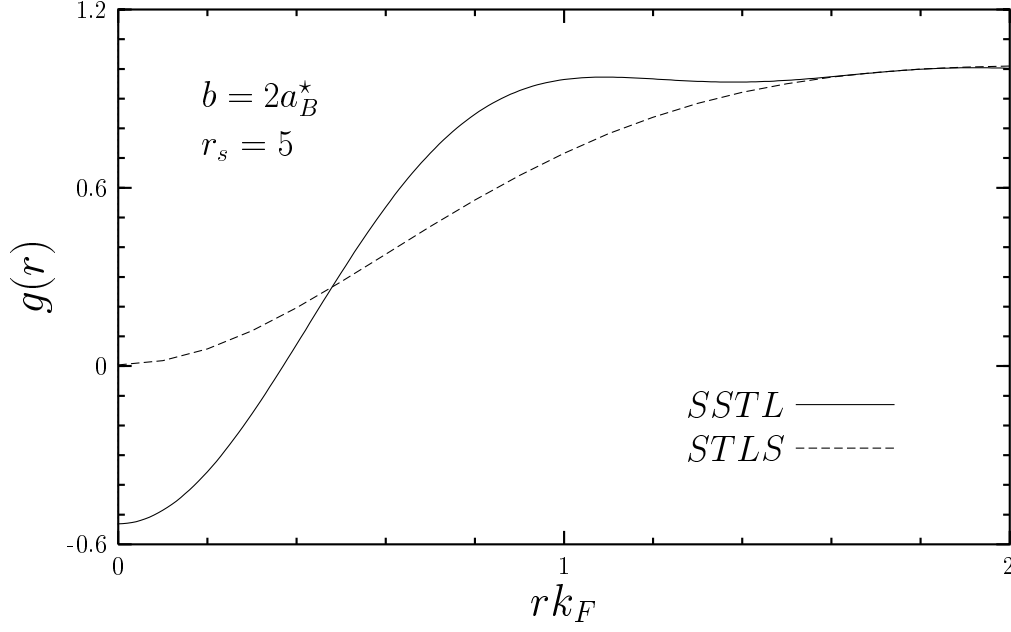


Figure 3: The pair correlation function in SSTL and STLS approximations for wire radius $b = 2a_B^*$ and $r_s = 5$.

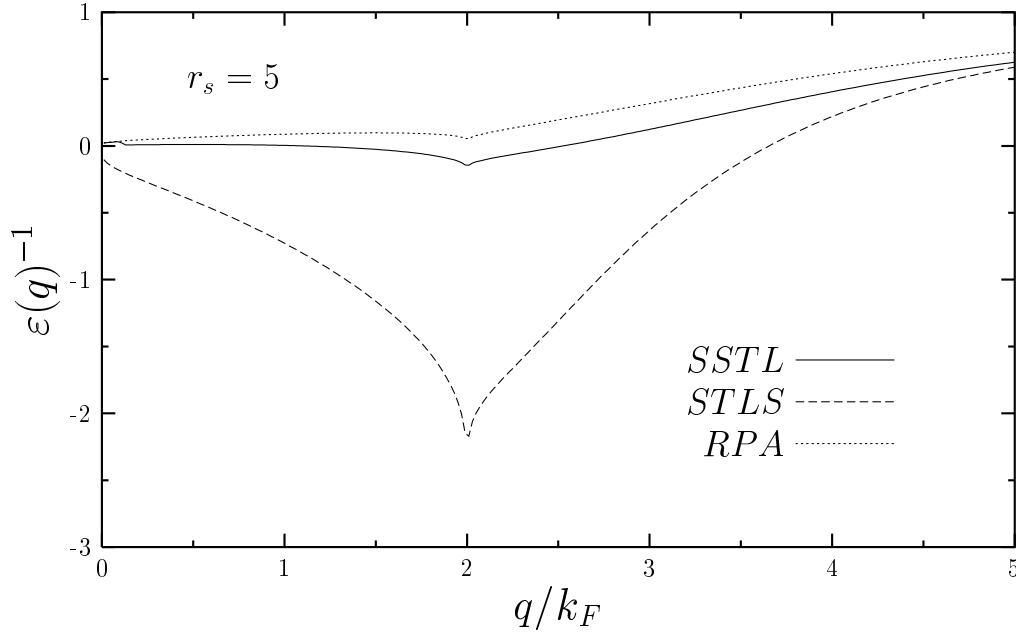


Figure 4: The inverse dielectric function in different approximations for wire radius $b = 5a_B^*$ and $r_s = 5$.

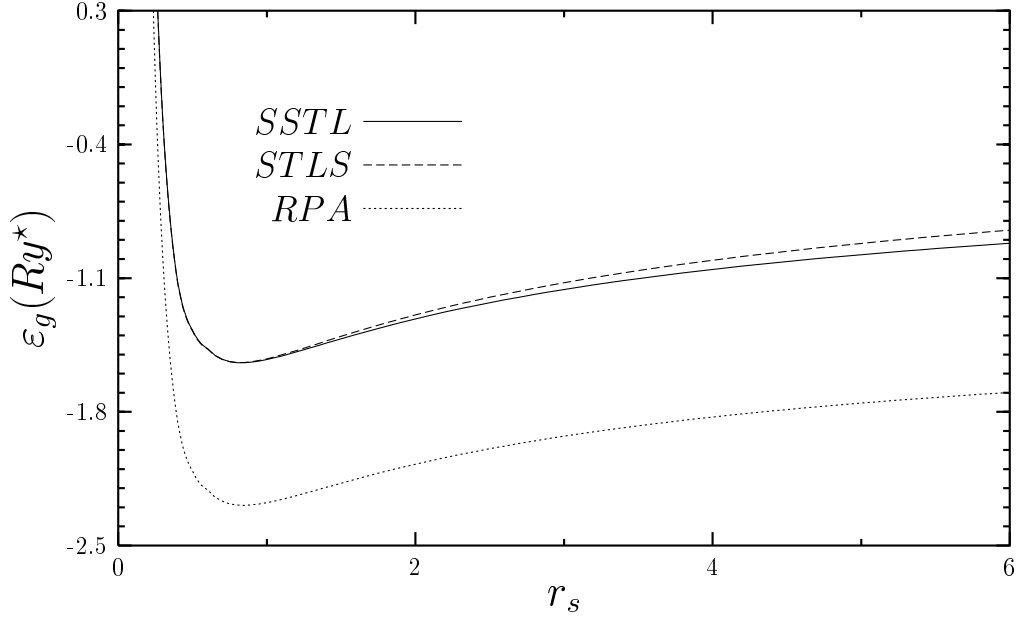


Figure 5: The ground state energy per particle in different approximations for wire radius $b = 2a_B^*$.

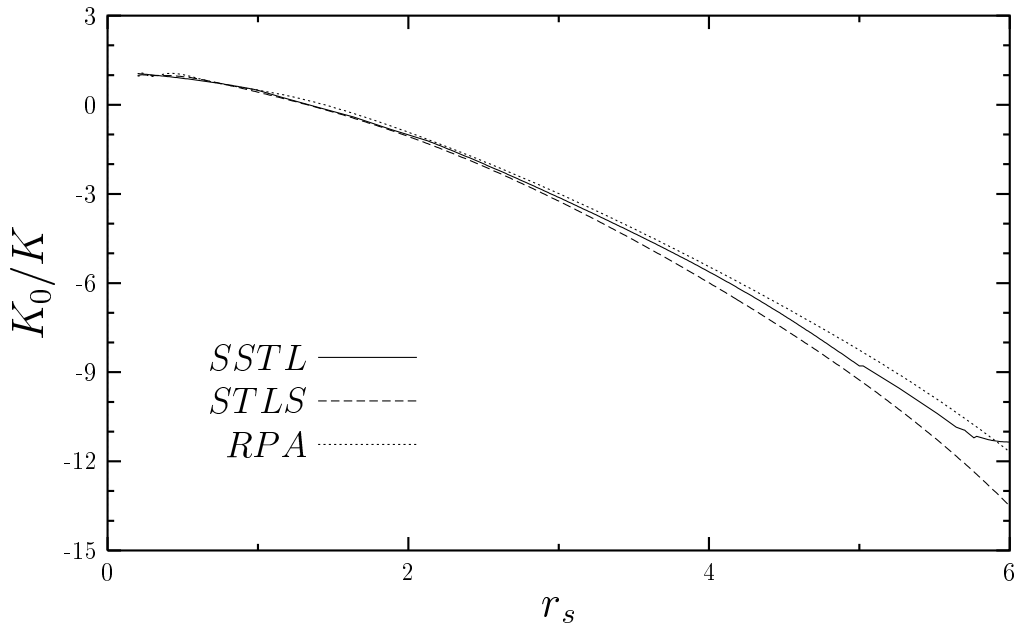


Figure 6: The compressibility calculated by using the ground state energy in three different approaches for wire radius $b = 2a_B^*$. Hereafter, K_0 is the free electron compressibility.

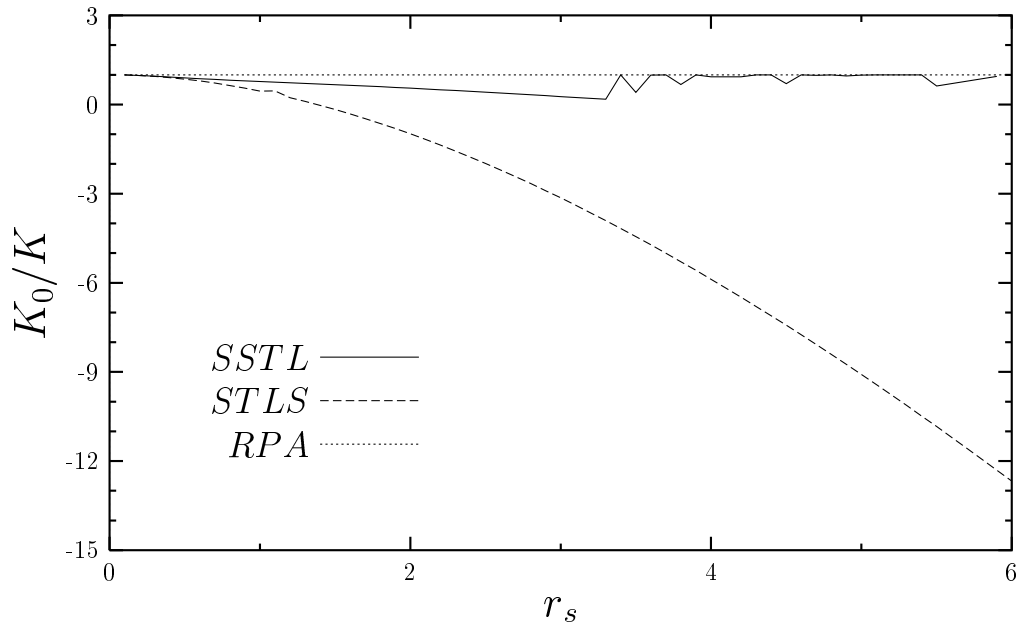


Figure 7: The compressibility calculated by using the $\lim_{q \rightarrow 0} \varepsilon(q, 0)$ in three different approaches for wire radius $b = 2a_B^*$.