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One-dimensional electron gas with short-range interaction: local-field correction and critical exponents

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Abstract. We study the one-dimensional electron gas with parabolic dispersion and a repulsive delta-function interaction potential. Using the ladder theory we obtain analytical results for the ground-state energy and the compressibility which are in agreement with exact results for weak and strong coupling. We calculate the short- and the long-distance behaviour of the pair-correlation function $g(z)$ and derive critical exponents from $g(z \rightarrow \infty)$. We evaluate the connection between the local-field correction and critical exponents.

1. Introduction

The mean-field theory is the basic theory to treat interaction effects [1]. The understanding of many-body effects going beyond the mean-field theory is one of the major topics in solid-state physics [2]. For the three-dimensional electron gas the concept of the so-called local-field correction was found to describe electronic properties of simple metals where many-body effects are already very important due to the large Wigner–Seitz radius [3]. The theory of Singwi, Tosi, Land, and Sjölander (STLS) [4] is a self-consistent theory for the local-field correction which is directed to understand the *short-distance behaviour* of the pair-correlation function which determines the ground-state energy. Within the STLS approach the local-field correction is independent of frequency. Recent theoretical [5] and experimental work [6] is directed towards understanding the frequency dependence of the local-field correction for the three-dimensional electron gas with Coulomb interaction.

In recent years [7] many-body effects have been studied for models where exact results can be obtained (for instance the one-dimensional Hubbard model). Perturbative renormalization-group theory [8], bosonization techniques [9], and the conformal field theory [10] were used and to get insight into the *long-distance behaviour* of correlation functions.

In this paper we study the pair-correlation function $g(z \rightarrow 0)$, which determines the ground-state energy, and $g(z \rightarrow \infty)$, which determines critical exponents, for a one-dimensional electron gas with a short-range interaction and we derive analytical results. The exact ground-state energy of this model has been calculated before [11, 12]. We show how to relate the ‘older’ many-body theory (using the concept of the local-field correction) with more ‘recent’ work in this field (using the renormalization group and bosonization techniques). As theory we apply the ladder theory [13].

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The paper is organized as follows. In section 2 we describe the model and the theory. The analytical results for the ground-state energy and the compressibility are given in section 3. In section 4 we discuss the local-field correction. The pair-correlation function and the critical exponents are calculated in section 5. A short discussion of our results is in section 6. We conclude in section 7.

2. Model and theory

We study a one-dimensional electron model with kinetic energy, characterized by an effective mass m (with parabolic dispersion $\varepsilon(q) = q^2/2m$), and interaction energy characterized by the potential V_0 (and the interaction potential between two particles at r_1 and r_2 is given by $V(r_1, r_2) = V_0\delta(r_1 - r_2)$). In the Fourier space the interaction potential is independent of the wavenumber q and expressed as $V(q) = V_0$. The electron density n , the electron mass, and V_0 define the relevant dimensionless parameter γ for the strength of the interaction as $\gamma \equiv mV_0/n = \pi V_0/2v_F$. $v_F = k_F/m$ is the Fermi velocity. The parameter $C_p = 2\gamma/\pi$ was introduced earlier [12, 13]. The electron density defines the Fermi wavenumber k_F via $n = 2k_F/\pi$. $\rho_F = n/2\varepsilon_F$ is the density of states at the Fermi energy ε_F . We express all results as functions of γ and we use $\hbar = 2\pi$.

The ladder theory was originally formulated for the long-range Coulomb potential [14, 15]. By summing up an infinite series of particle–particle ladder interactions, the pair-correlation function, which is positive for all coupling strength, has been obtained. In the ladder theory the effective interaction $I(\mathbf{p}, \mathbf{p}', \mathbf{q})$ between two electrons with wavenumber \mathbf{p} and \mathbf{p}' is given by the solution of the integral equation [14]

$$I(\mathbf{p}, \mathbf{p}', \mathbf{q}) = V(\mathbf{q}) + \sum_{\mathbf{k}} \frac{V(\mathbf{q} - \mathbf{k})[1 - n(\mathbf{q} + \mathbf{k})][1 - n(\mathbf{p}' - \mathbf{k})]}{\varepsilon(\mathbf{p}) - \varepsilon(\mathbf{p} + \mathbf{k}) + \varepsilon(\mathbf{p}') - \varepsilon(\mathbf{p}' - \mathbf{k})} I(\mathbf{p}, \mathbf{p}', \mathbf{k}) \quad (1)$$

where $V(\mathbf{q})$ is the Fourier transform of the interaction potential and $n(\mathbf{p})$ is the zero temperature Fermi distribution function. We are interested in the short-range behaviour of the system: in the following we apply the approximation $I(\mathbf{p}, \mathbf{p}', \mathbf{q}) = I(\mathbf{0}, \mathbf{0}, \mathbf{q})$ as used for the long-range Coulomb potential [14, 15]. In fact, the comparison of our approximation with the exact ladder theory [13] allows us to get some insight into this approximation which is always made for long-range potentials. For the short-range interaction potential we find that $I(\mathbf{0}, \mathbf{0}, \mathbf{q})$ is independent of the wavenumber: $I \equiv I(\mathbf{0}, \mathbf{0}, \mathbf{q})$. By defining $\Gamma \equiv mI/n$ we get

$$\Gamma = \frac{\gamma}{1 + 2\gamma/\pi^2} \quad (2)$$

where Γ decreases as $\Gamma = \gamma$ for $\gamma \rightarrow 0$ and saturates at $\Gamma = \pi^2/2$ for $\gamma \rightarrow \infty$. With $I(\mathbf{p}, \mathbf{p}', \mathbf{q})$ the pair-correlation function $g(z)$ can be calculated. Within the approximation $I(\mathbf{p}, \mathbf{p}', \mathbf{q}) = I(\mathbf{0}, \mathbf{0}, \mathbf{q})$ the pair-correlation function is given by [14]

$$g(0) = \frac{2}{n^2} \sum_{\mathbf{p}\mathbf{p}'} n(\mathbf{p})n(\mathbf{p}') \left[1 - \frac{1}{2} \sum_{|\mathbf{q}| > k_F} I(\mathbf{0}, \mathbf{0}, \mathbf{q})/\varepsilon(\mathbf{q}) \right]^2 \quad (3a)$$

where $g(z)$ is defined by $g(z) = [g_{\uparrow\uparrow}(z) + g_{\uparrow\downarrow}(z)]/2$ and can be expressed in terms of the static structure factor, see equation (11). With $g_{\uparrow\uparrow}(z=0) = 0$ (Pauli principle) this means that $g(0)$ is determined by the static structure factor for antiparallel spin configurations. For details of the ladder theory we refer to [14].

We obtain with equation (2) and equation (3a) the analytical result

$$g(0) = 1/[2(1 + 2\gamma/\pi^2)^2] \quad (3b)$$

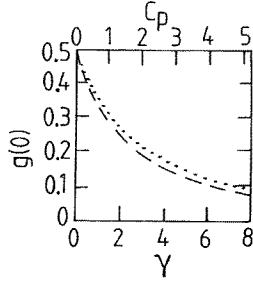


Figure 1. The pair-correlation function $g(z = 0)$ versus interaction strength γ (or C_p) according to equation (3b) is shown by the broken curve. The dotted curve represents numerical results within the exact ladder theory [13].

with $g(0) = (1 - 4\gamma/\pi^2)/2$ for $\gamma \rightarrow 0$ and $g(0) = \pi^4(1 - \pi^2/\gamma)/8\gamma^2$ for $\gamma \rightarrow \infty$. The comparison of $g(0)$ obtained within the ‘approximative’ ladder theory in equation (3b) with the ‘exact’ ladder theory [13] shows that our values of $g(0)$ are slightly smaller, see figure 1.

3. Ground-state energy and compressibility

The interaction energy $\varepsilon_{\text{int}}(\gamma)$ is given in terms of the static structure factor [2]. The static structure factor is related to the pair-distribution function $g(z)$ and one finds $\varepsilon_{\text{int}}(\gamma) = n^2\gamma g(0)/2m$ [13]. The contribution of the interaction energy ε_{int} to the ground-state energy ε_g per particle is expressed as

$$\varepsilon_{\text{int}} = \int_0^\gamma d\lambda \frac{\varepsilon_{\text{int}}(\lambda)}{\lambda}. \quad (4)$$

The contribution of the kinetic energy ε_{kin} to the ground-state energy per particle is given by $\varepsilon_{\text{kin}} = n^2\pi^2/24m$. The ground-state energy is written as

$$\varepsilon_g = \frac{n^2}{2m} \left[\frac{\pi^2}{12} + \int_0^\gamma d\lambda g(0) \right] \quad (5)$$

and the total energy is $E_g = n\varepsilon_g$. Within the ‘approximative’ ladder theory the total energy is given by the analytical expression

$$\frac{E_g}{\varepsilon_F k_F} = \frac{2}{3\pi} + \frac{4}{\pi^3} \frac{\gamma}{(1 + 2\gamma/\pi^2)}. \quad (6)$$

With (6) we derive for weak coupling $E_g/\varepsilon_F k_F = 2(1 + 6\gamma/\pi^2 - 12\gamma^2/\pi^4)/3\pi$ and for strong coupling $E_g/\varepsilon_F k_F = 8(1 - 3\pi^2/8\gamma)/3\pi$. We note that the Hartree–Fock (HF) and exchange (ex) energy is written as $\varepsilon_{\text{HF}} = \gamma n^2/4m = -\varepsilon_{\text{ex}}$ and the correlation (cor) energy is given by $\varepsilon_{\text{cor}} = -\gamma^2 n^2/[2m(\pi^2 + 2\gamma)]$ with $\varepsilon_{\text{cor}}/\varepsilon_{\text{ex}} = 1$ for $\gamma \rightarrow \infty$.

The weak-coupling result was calculated within the mean-field approximation [12, 13]. The exact strong-coupling result for $\gamma \rightarrow \infty$ corresponds to non-interacting spinless fermions with $E_g(\gamma \rightarrow \infty) = 4E_g(\gamma = 0) = 8\varepsilon_F k_F/3\pi$ with k_F replaced by $2k_F$ [12, 15]. The same ground-state energy was found in the strong-coupling limit of a Bose condensate in one dimension [16]. We conclude that the approximative ladder approach describes correctly the weak- and strong-coupling behaviour. For intermediate coupling our ground-state energy is about 5% lower than the exact result, see figure 2. This is the price we have to pay in order to get *analytical results*. The exact ladder theory [13] gives $E_g/\varepsilon_F k_F = 9.71/3\pi$ for $\gamma \rightarrow \infty$.

The compressibility κ can be expressed by the second derivative of the ground-state energy as $\partial^2 E_g/\partial n^2 = \pi v_F \kappa_0/2\kappa$ with $\kappa_0 = 4m/\pi^2 n^3$ as the compressibility of the free

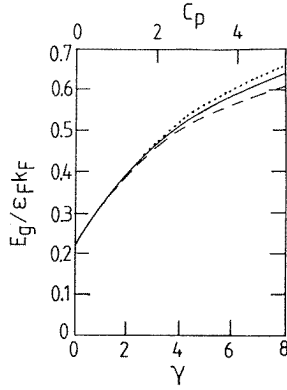


Figure 2. The total energy ε_{tot} (normalized to $\varepsilon_F k_F$) versus interaction strength γ (or C_p) according to equation (6) is shown by the broken curve. The full curve represents the exact result [12]. The dotted curve represents numerical results within the exact ladder theory [13].

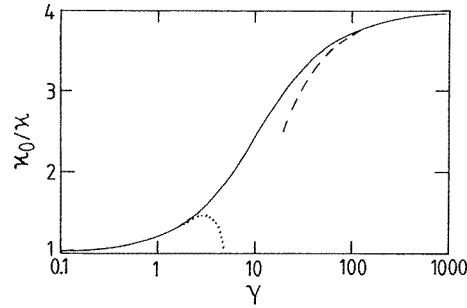


Figure 3. The inverse compressibility $1/\kappa$ (in units of the inverse compressibility of the free electron gas $1/\kappa_0$) according to equation (7). The broken and chain curves correspond to the asymptotic results.

electron gas [1]. With equation (6) we find

$$\frac{\kappa_0}{\kappa} = 1 + \frac{2\gamma}{\pi^2} \frac{1 + 6\gamma/\pi^2 + 12\gamma^2/\pi^4}{(1 + 2\gamma/\pi^2)^3}. \quad (7)$$

The asymptotic results are written as $\kappa_0/\kappa = 1 + 2\gamma/\pi^2 - 16\gamma^4/\pi^8$ for $\gamma \rightarrow 0$ and $\kappa_0/\kappa = 4(1 - 3\pi^2/4\gamma)$ for $\gamma \rightarrow \infty$, see figure 3. Note the large validity range of the weak coupling result in figure 3: $\gamma \leq 3$.

With the ground-state energy we can calculate the chemical potential μ as $\mu/\varepsilon_F = 1 + 4\gamma(1 + 3\gamma/\pi^2)/[\pi^2(1 + 2\gamma/\pi^2)^2]$, the kinetic energy t per particle as $t/\varepsilon_F = (1 + 4\gamma/\pi^2 + 16\gamma^2/\pi^4)/[3(1 + 2\gamma/\pi^2)^2]$ and the potential energy v per particle as $v/\varepsilon_F = 2\gamma/[\pi^2(1 + 2\gamma/\pi^2)^2]$. Note that $v = 0$ and $t = \varepsilon_F/3$ for $\gamma = 0$. For $1/\gamma = 0$ one finds $v = 0$ and $t = 4\varepsilon_F/3$. We conclude that for $1/\gamma = 0$ interaction effects disappear and the particles behave as free particles [12, 15].

4. Local-field correction

We define the local-field correction $G(q, \omega)$ by the dynamic density response function $X(q, \omega)$ as [2]

$$\mathbf{X}(q, \omega) = \frac{\mathbf{X}_0(q, \omega)}{1 + V_0[1 - G(q, \omega)]\mathbf{X}_0(q, \omega)}. \quad (8)$$

$\mathbf{X}_0(q, \omega)$ is the Lindhard function of the free-electron gas. Note that the local-field correction depends on q and ω . By using the compressibility sum-rule $\mathbf{X}(q \rightarrow 0, \omega = 0) \equiv \mathbf{X}(q \rightarrow 0) = n^2\kappa$ one finds [13]

$$G(0, 0) = 1 - \pi^2(\kappa_0/\kappa - 1)/4\gamma. \quad (9a)$$

With the analytical expression for κ_0/κ in equation (7) we derive

$$G(0, 0) = \frac{1 + 6\gamma/\pi^2 + 12\gamma^2/\pi^4 + 16\gamma^3/\pi^6}{2(1 + 2\gamma/\pi^2)^3} \quad (9b)$$

with $G(0, 0) = (1 + 8\gamma^3/\pi^6)/2$ for $\gamma \rightarrow 0$ and $G(0, 0) = 1 - 3\pi^2/4\gamma + 3\pi^4/16\gamma^2$ for $\gamma \rightarrow \infty$. From the high-frequency expansion of $\mathbf{X}(q, \omega)$ and by calculating ω -moments [4] of $\mathbf{X}(q, \omega)$ one gets [13]

$$G(q, \infty) = 1 - g(0). \tag{10a}$$

With equation (3b) we conclude that

$$G(q, \infty) = \frac{1 + 8\gamma/\pi^2 + 8\gamma^2/\pi^4}{2(1 + 2\gamma/\pi^2)^2} \tag{10b}$$

with $G(q, \infty) = (1 + 4\gamma/\pi^2 - 16\gamma^4/\pi^8)/2$ for $\gamma \rightarrow 0$ and $G(q, \infty) = 1 - \pi^4/8\gamma^2 + \pi^6/8\gamma^3$ for $\gamma \rightarrow \infty$.

The collective modes are given as the poles of $\mathbf{X}(q, \omega)$. With $\mathbf{X}_0(q, \omega \rightarrow \infty) \propto -q^2/\omega^2$ and $G(0, 0)$, in order to get the long wavelength limit of the collective density (d) modes, we find [17–19] $\omega_d(q)/v_F|q| = [\rho_F/\mathbf{X}(q \rightarrow 0)]^{1/2} = [\kappa_0/\kappa]^{1/2}$ with $\omega_d(q)/v_F|q| = 1 + \gamma/\pi^2 - \gamma^2/2\pi^4$ for $\gamma \rightarrow 0$ and $\omega_d(q)/v_F|q| = 2(1 - 3\pi^2/8\gamma)$ for $\gamma \rightarrow \infty$. For the velocity of sound v_d , using $\omega_d(q \rightarrow 0) = v_d|q|$, we find $v_d = v_F[\kappa_0/\kappa]^{1/2}$ [1].

5. Pair-correlation function and critical exponents

The pair-correlation function $g(z)$ is given by the static structure factor [2] and is expressed as

$$g(z) = 1 - \frac{1}{\pi n} \int_0^\infty dq \cos(qz)[1 - S(q)] \tag{11}$$

and $S(q)$ is the frequency integral over the dynamical structure factor $S(q, \omega)$. One can show that $g(z \rightarrow 0) = g(0) + g'(0)|z|$ with $g'(0) = A/2n$ [13] and A is given by

$$A = \lim_{q \rightarrow \infty} \{q^2[1 - S(q)]\}. \tag{12}$$

For small distances, following Kimball [20], the effective two-electron wavefunction $\varphi(z)$ is given by $\varphi(z \rightarrow 0) = \exp(\gamma k_F|z|/\pi)$ and one can establish a relation between $g(0) = |\varphi(z \rightarrow 0)|^2$ and $g'(0) = \partial|\varphi(z \rightarrow 0)|^2/\partial z : g'(0) = mV_0g(0)$. We derive the Kimball relation

$$g(0) = \frac{1}{2n^2\gamma} \lim_{q \rightarrow \infty} \{q^2[1 - S(q)]\} \tag{13}$$

and it follows the exact result

$$g(z \rightarrow 0) = g(0)[1 + \gamma n|z| + O(z^2)]. \tag{14}$$

In [21] we discussed the STLS approach for a long-range Coulomb potential with the static structure factor given by a generalized Feynman–Bijl (GFB) form. In the ladder theory the local-field correction depends on q and ω and the static structure factor in the GFB form must be generalized. We propose

$$S_{\text{GFB}}(q) = \frac{1}{[1/S_0(q)^2 + 4n^2\gamma[1 - G(q, \omega_1)]/q^2]^{1/2}} \tag{15}$$

where $S_0(q)$ is the static structure factor of the free-electron gas (particle–hole excitations). The term containing γ represents the collective modes and ω_1 is a characteristic frequency. With $S_0(q \geq 2k_F) = 1$ we conclude that $S_{\text{GFB}}(q \rightarrow \infty) = 1 - 2n^2\gamma[1 - G(q, \omega_1)]/q^2$ fulfils the Kimball relation in equation (13) if $1 - G(q, \omega_1) = g(0)$. For $g(z \rightarrow 0)$ we

conclude that $G(q, \omega_1)$ in equation (15) must be replaced by $G(q, \infty)$, see equation (10a). For $g(z \rightarrow \infty)$ we suggest that $G(q, \omega_1)$ in equation (15) should be replaced by $G(0, 0)$: this is in agreement with the bosonization approach [9] where the long wavelength and low-energy behaviour is used to characterize the system. With equation (11) we find for $g(z \rightarrow \infty)$ the analytical result

$$g(z \rightarrow \infty) = 1 - \frac{K_d}{(zn\pi)^2} [1 - K_d^2 \cos(2k_F z) + O(1/z^2)] \tag{16a}$$

with

$$K_d = \frac{1}{[1 + 4\gamma[1 - G(0, 0)]/\pi^2]^{1/2}} \tag{16b}$$

where K_d determines the long-distance decay of the pair-correlation function. With the compressibility sum rule in equation (9a) $K_d(\gamma)$ is written as

$$K_d = [\kappa/\kappa_0]^{1/2}. \tag{17}$$

In the weak-coupling limit we find $K_d = 1/(1 + 2\gamma/\pi^2 - 16\gamma^4/\pi^8)^{1/2} \approx 1 - V_0/2\pi v_F$ and for strong coupling $K_d = 1/(2 - 3\pi^2/8\gamma)$. For the Hubbard model, characterized by U and t , one gets $K_d(U/t \rightarrow 0) = 1 - U/\pi v_F$ and $K_d(U/t \rightarrow \infty) = 1/2$ with $v_F = 2t \sin(\pi\tilde{n}/2)$ and \tilde{n} is the band-filling factor [17,18]. The definition of the compressibility implies $\partial^2 E_g/\partial n^2 = \pi v_F \kappa_0/2\kappa$ [1]. With $\partial^2 E_g/\partial n^2 = \pi v_d/2K_d$ [18] we conclude that $K_d = (\kappa/\kappa_0)^{1/2}$. This result agrees with our equation (17) which was obtained from $g(z \rightarrow \infty)$.

K_d describes the singularity in the momentum distribution function by $n(k) = 0.5 - \text{const} \text{sign}(k - k_F)|k - k_F|^\alpha$ with $\alpha = [K_d^{1/2} + 1/K_d^{1/2} - 2]/4$ [18,22] and the density of states $\rho(\varepsilon)$ near the Fermi energy is expressed as $\rho(\varepsilon) \approx |\varepsilon - \varepsilon_F|^\alpha$ [22]. With equation (17) we obtain

$$\alpha = [(\kappa/\kappa_0)^{1/2} + (\kappa_0/\kappa)^{1/2} - 2]/4. \tag{18}$$

In figure 4 we show α versus γ . We conclude that $0 \leq \alpha \leq 1/8$ in agreement with results found for the Hubbard model [18,22,23].

We find in the weak-coupling limit

$$\alpha = \gamma^2(1 - 2\gamma/\pi^2)/4\pi^4. \tag{19a}$$

In the strong-coupling limit we get

$$\alpha = (1 - 9\pi^2/8\gamma)/8. \tag{19b}$$

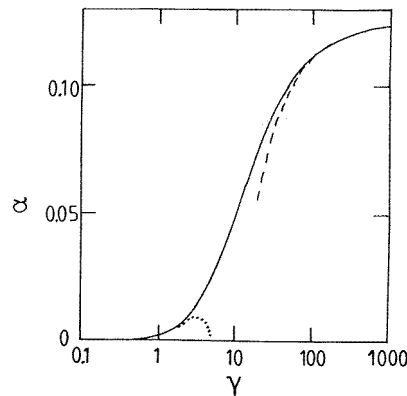


Figure 4. The critical exponent α versus interaction strength γ according to equation (18). The broken and chain curves correspond to the asymptotic results, see equation (19).

We note the large validity range of the weak-coupling result: $\gamma < 3$, see figure 4. Within the STLS approach [24] we found for weak coupling $\alpha_{\text{STLS}} = \gamma^2/4\pi^4$ † and for strong coupling $\alpha_{\text{STLS}} = 0.025$. In order to calculate the numerical factor $1/4\pi^4$ of α for weak coupling it is essential to know that no γ^2 -term exists in $\kappa_0/\kappa = 1 + 2\gamma/\pi^2 - 16\gamma^4/\pi^8$ for $\gamma \rightarrow 0$, see equation (7). Therefore, we believe that equation (19a) is a very important result of the present paper. We are not aware that an analytical result of α for weak coupling has already been published.

6. Discussion

It is a very surprising result of the present paper that, for the one-dimensional electron gas, analytical results for the ground-state energy can be obtained which are correct in the weak-coupling and strong-coupling limit. With the ground-state energy all related properties can be calculated. The novel result of the present paper is the fact that analytical results have been obtained.

In [13] the ladder theory was applied to calculate the ground-state energy directly and the two functions $A(\mathbf{p}, \mathbf{p}')$ and $h(x, y)$ were introduced. Without going into details we mention that our approximation corresponds to $A(\mathbf{p}, \mathbf{p}') = A(\mathbf{0}, \mathbf{0}) = -\rho_F/2$ and $h(x, y) = h(0, 0) = 1/\pi$. It should also be mentioned that the ladder theory had been applied before to the Hubbard model [25]. For a review, see [26].

From our theoretical results obtained in this paper we suggest that conventional many-body theory, developed for the three-dimensional electron gas with long-range Coulomb interaction [14] works quite well to describe the one-dimensional electron gas [13]. The concept of the local-field correction is an important concept even for the one-dimensional electron gas. This is of interest because many-body effects in the three-dimensional electron gas, where exact results are not available, are described by the local-field correction. We mention that many-body effects in the one-dimensional electron gas with a long-range Coulomb interaction have recently been discussed using the local-field correction [27].

Concerning experiments it should be noted that our theory contains collective modes and (one-particle) electron-hole excitations, see equation (8). Some recent experiments made with quantum wires [28–30] have shown that one-particle excitations exist. This is in agreement with our theory. In the bosonization approach [8, 9] such excitations do not exist.

7. Conclusion

We presented analytical results for the ground-state energy and the compressibility of a one-dimensional electron gas with short-range interaction as a function of the coupling parameter γ . Our calculation of $g(z \rightarrow \infty)$ shows that the critical exponent K_d is described by the local-field correction $G(0, 0)$. For $g(z \rightarrow 0)$ we found that $G(q, \infty)$ enters the Kimball relation. These results connect the ‘older’ many-body theory using the local-field correction with the ‘recent developments’ of the many-body theory using bosonization techniques and the renormalization group. Numerical and analytical results for the parameter α as a function of γ have been given.

† The weak coupling result in [24] should read $\alpha = \gamma^2/4\pi^4$.

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