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Some properties of short-range correlations for electrons in quantum wires

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Abstract

The asymptotic behaviours of the momentum distribution, the static structure factor and the local field factor at large momenta are evaluated for the jellium model of an interacting electron fluid confined in a quantum wire. The dependence of the results on the character of the confinement and their relevance to models of the dielectric screening function are discussed.

1. Introduction

Recent developments in fabrication techniques of quantum wires have made available for experimental study systems in which the conduction electrons can be described by a quasi-one-dimensional Fermi liquid (1DEL) model [1, 2]. The role of the electron–electron interactions in determining the observed electronic excitation spectra in these systems has been accounted for within the random phase approximation (RPA: see Ref. [3] and references given therein).

In such quantum wires the many-body effects are still small, because of the relatively high effective electron density and the relative large effective wire radius. One may expect, however, that with further developments in the production of semiconductor wire structures these system parameters may be varied into a range where the short-range electron–electron correlations that are neglected in the RPA would become relevant.

In the present paper we study some exact asymptotic behaviours of short-range correlations in a 1DEL. Specific attention is given to the behaviour of the momentum distribution at high momenta and to those of the structure factor and of the local field factor in dielectric screening at high wave numbers. Our approach is taken from earlier work on three-dimensional (3D) and two-dimensional (2D) electron liquids [4]. The results emphasize the dependence of short-range correlations in a 1DEL on the nature of the confinement.

2. The model

We consider a quantum wire of length L extending in the $\hat{z}$ direction. It contains N electrons which are free to move along the wire axis in the effective mass sense, but are confined in the $\hat{x}$–$\hat{y}$ plane by a potential well $U_c(x/a_x, y/a_y)$ where a_x and a_y are the characteristic lengths of the confinement along the $\hat{x}$ and $\hat{y}$ directions. The electronic system at zero temperature is characterized by an effective width

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R_0 and by the one-dimensional carrier density $\rho_\parallel = N/L$. All vectors will be decomposed into their in-plane and $\hat{z}$ components, with the notations $R \equiv (\boldsymbol{r}, z)$ for position vectors and $K \equiv (\boldsymbol{k}, k_z)$ for wave vectors.

The Hamiltonian H is the sum of a transverse part $H_\perp$, a longitudinal part $H_\parallel$ and the 3D electron–electron Coulomb interaction $V_{\text{e-e}}$: $H = H_\parallel + H_\perp + V_{\text{e-e}}$. The many-body wave function may be expanded in terms of the eigenfunctions ϕ_i of $H_\parallel$ and χ_j of $H_\perp$,

$$\Psi(R_1, \dots, R_N) = \sum_{i,j} C_{i,j} \phi_i(z_1, \dots, z_N) \chi_j(\boldsymbol{r}_1, \dots, \boldsymbol{r}_N). \quad (1)$$

If the combination of energy level spacing due to the confinement and linear carrier density is such that $\langle H_\perp \rangle \gg \langle V_{\text{e-e}} \rangle$, one may neglect any contribution from excited subband states. The wave function takes the form

$$\Psi(R_1, \dots, R_N) \approx \psi(z_1, \dots, z_N) \prod_i \chi(\boldsymbol{r}_i), \quad (2)$$

where $\psi(z_1, \dots, z_N) = \sum_i C_{i,0} \phi_i(z_1, \dots, z_N)$ and we have set $\chi_0(\boldsymbol{r}_1, \dots, \boldsymbol{r}_N) = \prod_i \chi(\boldsymbol{r}_i; a_x, a_y)$. The normalized single-particle ground state $\chi(\boldsymbol{r}_i; a_x, a_y)$ is completely determined by the confining potential. The electron density in the wire is then given by $\rho_w(R) = \rho_\parallel \rho_\perp(\boldsymbol{r})$, where $\rho_\perp(\boldsymbol{r}) = |\chi(\boldsymbol{r}; a_x, a_y)|^2$.

The approximation (2) allows one to formally define a purely one-dimensional jellium problem [5] in terms of the many-body wave function $\psi(z_1, \dots, z_N)$, the effective interactions in the limit $L \to \infty$ being weighted with $\rho_\perp(\boldsymbol{r})$ according to

$$v(k_z) = 2e^2 \int d^2\boldsymbol{r} \int d^2\boldsymbol{r}' \rho_\perp(\boldsymbol{r}) \rho_\perp(\boldsymbol{r}') K_0(k_z |\boldsymbol{r} - \boldsymbol{r}'|). \quad (3)$$

Here, $K_0(x)$ is the zeroth-order modified Bessel function of the second kind and $2e^2 K_0(k_z|a|)$ is the Fourier transform of $e^2/\sqrt{z^2 + a^2}$. We recall that $K_0(x) = -\ln(x)$ for $x \ll 1$ and $K_0(x) = \exp(-x)\sqrt{\pi/2x}$ for $x \gg 1$. For the 1DEL model we define the dimensionless length $r_s = (2\rho_\parallel a_0)^{-1}$ with a_0 the Bohr radius and the Fermi wave number $k_F = \pi\rho_\parallel/2$.

Eq. (3) can be rewritten as

$$v(k_z) = \frac{e^2}{\pi} \int \frac{|\rho_\perp(\boldsymbol{k})|^2}{k_z^2 + k^2} d^2\boldsymbol{k}, \quad (4)$$

where we have indicated with $\rho_\perp(\boldsymbol{k})$ the Fourier transform of $\rho_\perp(\boldsymbol{r})$. If both confinement lengths a_x and a_y are non-vanishing, and noticing that $\int |\rho_\perp(\boldsymbol{k})|^2 d^2\boldsymbol{k} = (2\pi)^2 \int |\rho_\perp(\boldsymbol{r})|^2 d^2\boldsymbol{r} < \infty$, we can use the dominated convergence theorem [6] to evaluate the asymptotic large-k_z behaviour of the integral in Eq. (4). We obtain

$$v(k_z) \to \frac{4\pi e^2}{k_z^2} Q_2, \quad (5)$$

where $Q_2 = \int |\rho_\perp(\boldsymbol{r})|^2 d^2\boldsymbol{r}$. However, if one of the confinement lengths (a_y say) vanishes, i.e. in the case $\rho_\perp(\boldsymbol{r}) = \rho_x(x)\delta(y)$ we can first perform the k_y integration in Eq. (4) and subsequently apply the dominated convergence theorem. We then obtain

$$v(k_z) \to \frac{2\pi e^2}{|k_z|} Q_1, \quad (6)$$

where $Q_1 = \int |\rho_x(x)|^2 dx$. We shall refer to these two cases in the following as a 3D-like and a 2D-like quantum wire and use them to emphasize the role of the type of confinement in determining the short-range correlations between the electrons.

3. The static structure factor

The pair distribution function $g_w(R_1, R_2)$ in the quantum wire is the probability of finding a pair of electrons at points R_1 and R_2, namely

$$g_w(R_1, R_2) = \frac{N(N-1)}{\rho_w(R_1)\rho_w(R_2)} \int |\Psi(R_1, \dots, R_N)|^2 \prod_{i=3}^N d^3R_i. \quad (7)$$

Upon inserting Eq. (2) in Eq. (7) we find the pair distribution function for the 1DEL,

$$g(z_1 - z_2) = \frac{N(N-1)}{\rho_\parallel^2} \int |\psi(z_1, \dots, z_N)|^2 \prod_{i=3}^N dz_i. \quad (8)$$

The static structure factor $S_w(K)$ of the quantum wire is related to the pair distribution function by

$$\begin{aligned} &\int [S_w(\boldsymbol{k}, k_z) - 1] \exp(-iK\,R) \frac{d^3K}{(2\pi)^3} \\ &= \frac{1}{\rho_\parallel} \int d^2\boldsymbol{r}_2 \rho_w(\boldsymbol{r}_2 + \boldsymbol{r}) \rho_w(\boldsymbol{r}_2) [g_w(R_2 + R, R_2) - 1] \\ &\equiv \frac{1}{\rho_\parallel} [G(R) - I(R)]. \end{aligned} \quad (9)$$

For the 1DEL we define $S(k_z) = S_w(0, k_z)$ so that Eq. (9) becomes

$$\int_{-\infty}^{\infty} [S(k_z) - 1] \exp(-\mathrm{i}k_z z) \frac{\mathrm{d}k_z}{2\pi} = \rho_\| [g(z) - 1]. \tag{10}$$

3.1. Large k_z behaviour in the 1DEL

Yasuhara [7] has shown for 3D jellium that the electron–electron ladder interactions at all orders determine the asymptotic form of the structure factor at large momenta. Following his method it is easily shown that $S(k_z)$ in the 1DEL has the following exact asymptotic form for large k_z ($k_z \gg k_F$):

$$1 - S(k_z) = \frac{v(k_z)}{\varepsilon(k_z)} \rho_\| g(0) + \cdots, \tag{11}$$

with $\varepsilon(k_z) = k_z^2/2m$. Therefore, if the 1DEL is confined in a 3D-like quantum wire, by inserting Eq. (5) in Eq. (11) we get

$$1 - S(k_z) = \frac{8\pi\rho_\|}{a_0} \frac{1}{k_z^4} Q_2 g(0) + \cdots. \tag{12}$$

If instead the 1DEL is confined in a 2D-like quantum wire we should use Eq. (6) in Eq. (11), thus obtaining

$$1 - S(k_z) = \frac{4\pi\rho_\|}{a_0} \frac{1}{|k_z|^3} Q_1 g(0) + \cdots. \tag{13}$$

The power law for the asymptotic approach of the structure factor to unity in Eq. (12) resembles that found by Kimball [8] for 3D jellium. Similarly, the form of Eq. (13) resembles that for 2D jellium [9].

3.2. Large k_z behaviour in a quantum wire

More generally, for a 3D quantum wire Eq. (9) yields

$$\lim_{t\to\infty} (tK)^4 [S_w(tk_x, tk_y, tk_z) - 1] = -8\pi\rho_\| \frac{\mathrm{d}}{\mathrm{d}|R|} [\hat{G}(|R|) - \hat{I}(|R|)] \Big|_{|R|=0}, \tag{14}$$

where $\hat{G}(|R|) - \hat{I}(|R|)$ is the average of $G(R) - I(R)$ taken over the sphere of radius $|R|$. The analogous expression for a 2D wire is

$$\lim_{t\to\infty} (tK)^3 [S_w(tk_x, tk_z) - 1] = -2\pi\rho_\| \frac{\mathrm{d}}{\mathrm{d}|R|} [\hat{G}(|R|) - \hat{I}(|R|)] \Big|_{|R|=0}. \tag{15}$$

Since $I(R)$ is completely determined from the knowledge of the confining potential, the same will be true for $(\mathrm{d}/\mathrm{d}|R|)\hat{I}(|R|)|_{|R|=0}$. On the other hand, $(\mathrm{d}/\mathrm{d}|R|)\hat{G}(|R|)|_{|R|=0}$ must be proportional to $G(0)$ as a consequence of the cusp theorem [10]. This yields

$$\frac{\mathrm{d}}{\mathrm{d}|R|} \hat{G}(|R|) \Big|_{|R|=0} = \frac{1}{a_0} G(0) \tag{16}$$

for a 3D-like wire and

$$\frac{\mathrm{d}}{\mathrm{d}|R|} \hat{G}(|R|) \Big|_{|R|=0} = \frac{2}{a_0} G(0) \tag{17}$$

for a 2D-like one.

4. The momentum distribution

The probability $n_w(K)$ of finding an electron with momentum K in the quantum wire, per unit transverse area, can be written as

$$n_w(K) = \rho_\| \int \exp[\mathrm{i}K(R - R')] \Psi^*(R, R_2, \ldots, R_N) \times \Psi(R', R_2, \ldots, R_N) \mathrm{d}R \, \mathrm{d}R' \prod_{i=2}^{N} \mathrm{d}R_i. \tag{18}$$

In the 1DEL approximation $n_w(K)$ takes the form

$$n_w(K) = |\phi(\boldsymbol{k})|^2 n(k_z) \tag{19}$$

where $\phi(\boldsymbol{k})$ is the Fourier transform of the single-particle ground state for the motion in the transverse direction and $n(k_z)$ is the momentum distribution in the 1DEL. From Eq. (2) we have

$$n(k_z) = \rho_\| \int \exp[\mathrm{i}k_z(z - z')] \psi^*(z, z_2, \ldots, z_N) \times \psi(z', z_2, \ldots, z_N) \mathrm{d}z \, \mathrm{d}z' \prod_{i=2}^{N} \mathrm{d}z_i. \tag{20}$$

4.1. Large k_z behaviour in the 1DEL

As was shown for 3D jellium by Yasuhara and Kawazoe [11], the electron–electron ladder diagrams also determine the asymptotic form of the momentum distribution at large momenta. We follow their approach for the one-electron momentum distribution in the 1DEL. It is easily shown that $n(k_z)$ has for large k_z ($k_z \gg k_F$) the asymptotic form

$$n(k_z) = \left(\frac{\rho_{\|} v(k_z)}{2\varepsilon(k_z)}\right)^2 g(0) + \cdots. \tag{21}$$

Therefore, if the 1DEL is confined in a 3D-like quantum wire, using Eq. (5) in Eq. (21) yields

$$n(k_z) = \left(\frac{4\pi\rho_{\|}}{a_0}\right)^2 \frac{1}{k_z^8} Q_2^2 g(0) + \cdots. \tag{22}$$

If instead the 1DEL is confined in a 2D-like quantum wire we should use Eq. (6) in Eq. (21), with the result

$$n(k_z) = \left(\frac{2\pi\rho_{\|}}{a_0}\right)^2 \frac{1}{k_z^6} Q_1^2 g(0) + \cdots. \tag{23}$$

The power-law decays of the momentum distribution in Eqs. (22) and (23) are the same as for 3D and 2D jellium. These were derived by Kimball [12] and by Rajagopal and Kimball [9], respectively, through an alternative argument that we apply to a quantum wire immediately below.

4.2. Large k_z behaviour in a quantum wire

The momentum distribution is obtained from Eq. (18) as the Fourier transform of a function which is bilinear in the many-electron wave function and its asymptotic form at large momenta is determined by the points of non-analyticity in the wave function. On the other hand, when two electrons are very close to each other their mutual repulsion dominates over the interactions with the other electrons and hence the dominant behaviour of the wave function can be determined from the two-body Schrödinger equation. Such a constraint implies that the many-electron wave function is everywhere continuous with its derivative excepts at points in phase space which correspond to zero interparticle separation.

By developing this argument, which is originally due to Kimball [12], we find

$$n_w(\boldsymbol{k}, k_z) \xrightarrow[\boldsymbol{k}\ \text{fixed}]{k_z \to \infty} \left(\frac{4\pi\rho_{\|}}{a_0}\right)^2 \frac{1}{k_z^8} \int |\rho_{\perp}(\boldsymbol{r})|^2 g_w(R, R)\, d\boldsymbol{r} \tag{24}$$

for a 3D-like quantum wire and

$$n_w(\boldsymbol{k}, k_z) \xrightarrow[\boldsymbol{k}\ \text{fixed}]{k_z \to \infty} \left(\frac{2\pi\rho_{\|}}{a_0}\right)^2 \frac{1}{k_z^6} \int |\rho_{\perp}(\boldsymbol{r})|^2 g_w(R, R)\, d\boldsymbol{r} \tag{25}$$

for a 2D-like one.

5. The local field factor

The linear density response function $\chi(k_z, \omega)$ of the 1DEL can be written in terms of the interacting reference susceptibility $\chi_I(k_z, \omega)$ and of a local field factor $\tilde{G}(k_z, \omega)$ as

$$\chi(k_z, \omega) = \frac{\chi_I(k_z, \omega)}{1 - v(k_z)[1 - \tilde{G}(k_z, \omega)]\chi_I(k_z, \omega)}. \tag{26}$$

The interacting reference susceptibility, first introduced by Niklasson [13] for 3D jellium, is defined in a similar way as the Lindhard free-electron response function but with the ideal Fermi momentum distribution replaced by the true momentum distribution of the interacting electron assembly.

Following the method used by Niklasson [13] it can be shown that for points in the (k_z, ω) plane well outside the region of particle–hole excitations, the local field factor in Eq. (26) satisfies two exact limiting behaviours. These are expressed in terms of the function

$$G^{PV}(k_z) = \frac{1}{2\pi\rho_{\|}} \int_{-\infty}^{\infty} dq \left\{ \frac{q^2 v(q)}{k_z^2 v(k_z)} - \frac{(q + k_z)^2 v(q + k_z)}{k_z^2 v(k_z)} \right\} [S(q) - 1]. \tag{27}$$

$G^{PV}(k_z)$ is the form taken in the 1DEL by the static local field factor first introduced by Pathak and Vashishta [14] for 3D jellium.

Niklasson's method involves a study of the equations of motion for the single-particle and the two-particle density matrices, which allow a full evaluation of the interacting reference susceptibility in the limit of large K or large ω. It is easily shown that the following limit must hold for $|\omega \pm k_z^2/2m| \gg k_F^2/2m$ and ω finite,

$$\lim_{k_z \to \infty} \tilde{G}(k_z, \omega) = G^{PV}(\infty). \tag{28}$$

Using Eqs. (5) and (6) in Eqs. (27) and (28) we find

$$\tilde{G}(k_z \to \infty, \omega) = 1 - g(0) + \frac{1}{8\pi^2 e^2 \rho_{\|} Q_2} \int \mathrm{d}q\, q^2 v(q) [S(q) - 1] \tag{29}$$

for a 1DEL obtained from 3D confinement and

$$\tilde{G}(k_z \to \infty, \omega) = 1 - g(0) \tag{30}$$

for a 1DEL with 2D confinement. Eq. (30) coincides with the result obtained by Santoro and Giuliani [15] for 2D jellium.

Finally, it is also easily shown by the same method that

$$\lim_{\omega \to \infty} \tilde{G}(k_z, \omega) = G^{PV}(k_z) \tag{31}$$

for $|\omega \pm k_z^2/2m| \gg k_F^2/2m$ and k_z finite.

A final remark concerning the asymptotic behaviour of static dielectric screening at large wave numbers is in order. After rewriting Eq. (26) in terms of the Lindhard function $\chi_0(k_z, \omega)$ and of a new local field factor $G(k_z, \omega)$,

$$\chi(k_z, \omega) = \frac{\chi_0(k_z, \omega)}{1 - v(k_z)[1 - G(k_z)\chi_0(k_z, \omega)]}, \tag{32}$$

it is easily shown from our results that $G(k_z, 0)$ increases as k_z^2 at large momenta in a 1DEL with 3D-like confinement and as $|k_z|$ when the confinement is 2D-like. These behaviours reproduce those first pointed out by Holas [16] for 3D and 2D jellium.

6. Concluding remarks

The Coulomb interaction potential between electrons in a quantum wire would not have a Fourier transform if both confinement lengths were taken as vanishingly small, because of its divergence at vanishing separation. The transverse density form factor $\rho_\perp(\boldsymbol{r})$, with Fourier transform $\rho_\perp(\boldsymbol{k})$, therefore is a crucial element of the theory and through it the nature of the confinement enters to determine the effective 1D electron–electron interaction in Eqs. (3) and (4). The Coulomb matrix element at large momentum transfers takes in general a 3D-like form as in Eq. (5), reducing to the 2D-like form of Eq. (6) in the case where one of the confinement lengths can be taken as vanishingly small. These asymptotic forms arise from transverse averaging of the Bessel function in the integrand in Eq. (3), which by itself would lead to an exponential decay factor at large momenta.

The asymptotic behaviours of the momentum distribution, the static structure factor and the local field factor that we have explicitly evaluated at large momenta reflect the above nature of the Coulomb matrix element. Dimensional cross-over in these behaviours is to be expected as one of the confinement lengths is squeezed down. Even in the case of 3D-like confinement, however, the short-range correlations reflect the confinement through the magnitude of the parameter Q_2.

References

[1] A.S. Plaut, H. Lage, P. Grambow, D. Heitmann, K. von Klitzing and K. Ploog, Phys. Rev. Lett. 67 (1991) 1642.

[2] A.R. Goñi, A. Pinczuk, J.S. Weiner, J.M. Calleja, B.S. Dennis, L.N. Pfeiffer and K.W. West, Phys. Rev. Lett. 67 (1991) 3298.

[3] Q.P. Li and S. Das Sarma, Phys. Rev. B 43 (1991) 11 768.

[4] K.S. Singwi and M.P. Tosi, Solid State Phys. 36 (1981) 177.

[5] W.I. Friesen and B. Bergersen, J. Phys. C 13 (1980) 6627.

[6] The dominated convergence theorem asserts that when integrating a sequence of pointwise convergent functions f_n it is permissible to bring the limit inside the integral sign if the absolute values of all the f_n are bounded from above by one integrable function. See W. Rudin, Real and Complex Analysis (McGraw-Hill, New York, 1966) p. 26.

[7] H. Yasuhara, Physica 78 (1974) 420.

[8] J.C. Kimball, Phys. Rev. A 7 (1973) 1648.

[9] A.K. Rajagopal and J.C. Kimball, Phys. Rev. B 15 (1977) 2819.
[10] A.E. Carlsson and N.W. Ashcroft, Phys. Rev. B 25 (1982) 3474 and references given therein.
[11] H. Yasuhara and Y. Kawazoe, Physica A 85 (1976) 416.
[12] J.C. Kimball, J. Phys. A 8 (1975) 1513.
[13] G. Niklasson, Phys. Rev. B 10 (1974) 3052.
[14] K.N. Pathak and P. Vashishta, Phys. Rev. B 7 (1973) 3649.
[15] G.E. Santoro and G.F. Giuliani, Phys. Rev. B 37 (1988) 4813.
[16] A. Holas, in: Strongly Coupled Plasma Physics, eds. F.J. Rogers and H.E. DeWitt (Plenum, New York, 1986) p. 463.