On the "effective exponent theory" of the Coulomb Luttinger liquid

Yasha Gindikin and V. A. Sablikov
Institute of Radio Engineering and Electronics, Russian Academy of Sciences, Fryazino, Moscow District, 141190, Russia

The "effective exponent theory", developed by Wang, Millis and Das Sarma in [Phys. Rev. B 69, 167101 (2004), Phys. Rev. B 64, 193307 (2001)], fails to calculate correctly the dynamic correlators of Coulomb Luttinger liquid. Main drawbacks are (i) cutting off the Coulomb potential by killing its long-range component, (ii) the absence of non-contradictory procedure to determine the 'scaling cutoff' and correlation functions for true Coulomb interaction.

I. INTRODUCTION

Wang, Millis and Das Sarma (WMS) proposed an 'effective exponent' approach to calculate the dynamic correlation functions in a Luttinger liquid with Coulomb interaction (CLL) and developed this theory in recent publications opposing it to our approach to the same problem. They claimed that (i) their method is 'more elementary' than our one, but is applicable in a wider energy range, (ii) both methods are equivalent in describing the threshold behavior of charge-density wave (CDW) structure factor and the dynamic spectral function (after a technical error in deriving the spectral function in our work has been eliminated). In this Comment, we show that:

i) The 'effective exponent theory' fails to take adequately into account the long-range nature of the Coulomb interaction and does not correctly describe the dynamic correlation functions.

ii) WMS's method contains a concealed procedure of fitting to the results of independent approaches and hence is not a self-sufficient theory. Correspondingly, the range of applicability of WMS's method is at least not wider than that of the reference approach.

iii) WMS's results for the CDW structure factor and spectral function disagree with our asymptotically exact results, and also contradict their own earlier numerical calculations. In particular, the ratio of two results for the spectral function ρ(q,ω) tends to infinity in the threshold region of δ ≡ ω - ωq-kF → +0 like exp[C ln δ^3/2], that is faster than any power of 1/δ.

The theory of WMS would not probably have been deserving a special discussion, if it had not involved an important physical problem of Coulomb interaction effects in low-dimensional electron systems and methods of its description.

Coulomb interaction effects are a rather complicated matter, studying which requires a delicate approach. The brash approximations can destroy the studied model so that it will be far from the realistic physical system. The analysis of the WMS theory is quite instructive to illustrate this. Their theory distorts strongly the Coulomb potential by killing its long-range component that is of most interest.

II. COULOMB INTERACTION PROBLEM

In principle, the Coulomb interaction problem is solved in the spinless Luttinger liquid theory. The bosonization method allows one to exactly calculate all the correlation functions for any type of the electron-electron interaction potential, and, in particular, does so for the long-ranged Coulomb interaction As a result, correlators are expressed in terms of definite integrals. Thus, the CDW structure factor SCDW(q,ω) equals

$$S_{CDW}(q,\omega) = \int_{-\infty}^{+\infty} dx e^{-iqx} \int_{-\infty}^{+\infty} dt e^{i\omega t} S(x,t), \quad (1)$$

with

$$S(x,t) = -\frac{1}{8\pi^2} q^2 \exp[-v_F \int_{-\infty}^{+\infty} \frac{dp}{\omega_p} \times \left(1 - e^{-i\omega t - ipx}) e^{-\alpha |p| \cos(2k_F x)} \right). \quad (2)$$

Here v_F is the Fermi velocity, ω_q = |q|v_F/g(q) is bosonic excitation spectrum, the interaction parameter g(q) is related to the Fourier-component of the interaction potential by g(q) = [1 + V(q)/\hbar\pi v_F]^{-1/2}.

Therefore, the task is reduced to the calculation of such integrals. However, in the case of Coulomb interaction such calculation entails serious mathematical difficulties that are connected inherently to the slow decrease of the interaction potential at large distances.

True Coulomb interaction is well known to be a special one. The distinctive feature of Coulomb interaction is that the integral of Coulomb potential

$$V(x) \approx e^2/\sqrt{x^2 + d^2}$$

diverges at large distance, d being the quantum wire diameter. Correspondingly, the Fourier-component of the potential goes to infinity in the long-wave limit q → 0 as

$$V(q) \sim 2e^2/|\ln qd|. \quad (3)$$

This manifests itself in the logarithmic divergency of the collective excitation velocity v(q) at q → 0. Any approximation of the Coulomb interaction by cutting off at large distance loses this feature and hence makes the interaction a non-Coulomb one.
The central question is whether long-ranged Coulomb interaction leads to a qualitatively new behavior of 1D electrons as compared to the short-ranged interaction case, which is easier to solve?

The classic paper of H.J. Schulz1 gave the positive answer to this question. Coulomb interaction was shown to have dramatic consequences for the density-density correlations of a 1D electron liquid. Specifically, the pair density correlator in the Coulomb case decays with the distance in the extremely slow fashion \(\exp[-c(\ln x)^{1/2}]\), instead of a power law, typical of the short-ranged interaction. In other words, in 1D systems Coulomb interaction induces a quasi-long-range order, close to the Wigner crystal.

Ref. 3 deals only with the static correlations. Dynamic correlations are much more difficult matter because the dependence on both \(q\) and \(\omega\) has to be addressed. Exact results are apparently of key importance in the exploration of this problem. They were not obtained until very recently.

The analytic approach to dynamic CLL correlators developed in our paper consists in the regular derivation of the integral equation for \(S_{\text{CDW}}(q,\omega)\) and \(\rho(q,\omega)\) and its solution near the threshold. What is important is that no model simplifications pertaining to the form of the Coulomb potential are used in this approach.

In WMS’s method,2 no Coulomb integrals are calculated analytically. WMS replaced the Coulomb interaction with an ‘effective’ short-ranged interaction, i.e. cut off the long-ranged Coulomb potential at large distance. Thus their approach is a model one. But this is not its major shortcoming. The real trouble lies in the arbitrariness of such replacement, as a consequence of which the authors, turning to their method in different publications, each time obtain different results. This becomes evident if one considers how Coulomb interaction is transformed into short-ranged one. Since WMS in their publications do not go into the details of such procedure, we briefly outline it here for the case of the CDW structure factor \(S_{\text{CDW}}(q,\omega)\).

### III. EFFECTIVE EXPONENT THEORY

WMS start2 with imposing the long-distance cutoff on the Coulomb potential at some wave-vector \(q_0\).

\[
V(q) = 2e^2|\ln((q_0+q)d)|. \tag{4}
\]

In contrast to Eq. (3), this potential does not diverge at \(q \to 0\), and hence is not the long-ranged Coulomb potential.

The structure factor \(S_{\text{CDW}}(q,\omega)\), having been calculated with the screened potential of Eq. (4), acquires the dependence on the cutoff parameter, i.e. \(S_{\text{CDW}}(q,\omega)\) is transformed into \(S_{\text{CDW}}(q_0,q,\omega)\). However, even for such cut off interaction no formulas are derived. Instead, the authors refer to common results for the short-ranged interaction, according to which

\[
S_{\text{CDW}}(q,\omega) \propto (\omega - \omega_{q-2k_F})^{\alpha_{\text{CDW}}} \tag{5},
\]

where the exponent equals \(\alpha_{\text{CDW}} = g(0) - 1\).

WMS ‘simply replace’ the Coulomb interaction parameter \(g(q) \sim |\ln|qd||^{-1/2} \) by \(g(q_0)\) and postulate that the ‘effective’ exponent equals

\[
\alpha_{\text{CDW}}(q_0) = g(q_0) - 1. \tag{6}
\]

Determining \(q_0\) is the main trouble of WMS’s approach. Indeed, no consistent theory exists until the procedure to determine \(q_0\) is defined. Assuming \(q_0\) constant (a fitting parameter) results in a standard power-law dependence of the structure factor \(S_{\text{CDW}}(q,\omega)\). For CLL, this corresponds neither to the numerical calculations nor the expectations, based on exactly solvable models. To obtain the formulas similar to those of Schulz, WMS subject \(S_{\text{CDW}}(q_0; q, \omega)\) to further modification by introducing the explicit dependence of \(q_0\) on \(q\) and \(\omega\). In other words, the cutoff parameter \(q_0\) is replaced by a function of two arguments \(q_0(q,\omega)\). Notice that introducing the cutoff \(q_0\), which depends on \(\omega\) and \(q\), can not be justified by any renormalization group arguments.

WMS propose no regular way to obtain the function \(q_0(q,\omega)\). Consequently, their method does not solve the Coulomb interaction problem. In fact, \(q_0\) is chosen from the intuitive conjectures, differently for different correlators being calculated. In the case of \(S_{\text{CDW}}(q,\omega)\), WMS postulate without convincing justification that \(q_0(q,\omega)\) is determined from the following equation,

\[
\omega_{q_0} = \omega - \omega_{q-2k_F}. \tag{7}
\]

In the case of \(\rho(q,\omega)\), they state that \(q_0(q,\omega)\) should be determined from other equation,

\[
\omega_{q_0} = \omega - \omega_{q-k_F}. \tag{8}
\]

In doing so, they ignore the fact that in both cases \(q_0(q,\omega)\) enters into the same expression for the potential in Eq. (4). As a result, the electron-electron interaction potential turns out to be different for different correlators. This ‘scaling cut-off’ procedure is seen to be physically inappropriate.

The most important problem WMS confront further is how to obtain the end result for correlation functions, even having the function \(q_0(q,\omega)\). In an earlier version of their theory, \(S_{\text{CDW}}\) was determined according to Eqs. (4), (5), (6), but this result did not satisfy the authors, and in the final release they declared another procedure. WMS postulated that the structure factor satisfies the following differential equation (see Eq. (14) of Ref. 3)

\[
\frac{\partial \ln S_{\text{CDW}}(\epsilon)}{\partial \ln \epsilon} = \alpha_{\text{CDW}}(q_0), \tag{9}
\]

where \(\epsilon\) denotes a normalized energy deviation from the threshold, \(\epsilon = (\omega - \omega_{q-2k_F})/\omega_0\), with \(\omega_0 = v_F/\beta d, \beta = [\pi v_F/2e^2]^{1/2}\).
Eq. (9) is seen to be a fundamental principle of the ‘effective exponent theory’, which allows WMS to find the dynamic structure factor analytically. However, no proof is provided that the structure factor, given by Eqs. 10-12, indeed satisfies this equation, at least asymptotically in the threshold region of $\epsilon \to 0$.

Solving Eq. (9), WMS obtain the following expression for $S_{CDW}$ (Eq. (15) of Ref. 3)

$$S_{CDW}(q, \omega) \propto \exp(-2\beta |\ln \epsilon|^{1/2})/\epsilon .$$

The asymptotically exact expression for $S_{CDW}(q, \omega)$ at $\epsilon \to 0$ was found in our paper.

$$S_{CDW}(q, \omega) \sim v_F e^{-4\beta |\ln \epsilon|^{1/2}}/\epsilon |\ln \epsilon|^{1/2} .$$

The comparison of the WMS result (Eq. (10)) with our result (Eq. (11)) via dividing one expression by another

$$S_{WMS} / S_{GS} \propto \exp(2\beta |\ln \epsilon|^{1/2})$$

shows that in the most interesting threshold region $\epsilon \to +0$, the ratio goes to infinity. This means that above results for the CDW structure factor are not equivalent, in contrast to what WMS stated. Possibly, one may invent some prescript to fit the effective exponent expression to the correct result but this hardly will be of interest.

Exactly the same steps are used in order to obtain the dynamic spectral function. The latest presentation of the effective exponent theory does not contain the explicit form of the spectral function. However, WMS’s strategy, as it is presented in Ref. 4, straightforwardly leads to the following expression,

$$\rho(q, \omega) \propto \exp(-1/6\beta |\ln \delta|^{3/2}) ,$$

which gives the threshold behavior of the CLL dynamic spectral function in the spinless case. Our result for the spectral function is derived below, see Eq. (19). In the threshold region $\delta \to +0$, the ratio

$$\rho_{WMS} / \rho_{GS} \propto \exp(1/6\beta |\ln \delta|^{3/2}) ,$$

goes to infinity faster than any power of $1/\delta$, which means that the results are incompatible.

It is interesting to note that the results of analytic effective exponent theory contradict WMS’s earlier numerical calculations also in the spinful case. Indeed, the analytic ‘effective exponent procedure’ of Ref. 3 gives in this case $\rho(q, \omega) \propto \exp(-1/6\beta |\ln \delta|^{3/2})$, whereas in Ref. 4 it was found that $\rho(q, \omega) \propto \exp(-1/6\beta |\ln \delta|^{3/2})$. The ratio of these expressions again goes to infinity in the threshold region as $\delta \to +0$.

The above examples show convincingly that the ‘effective exponent theory’ is a fitting to the independent (analytic or numerical) results, rather than a justified self-sufficient procedure. Consequently, the WMS claim that their ‘effective exponent theory’ applies over a much wider energy range than our method is misleading. The effective exponent theory can not give correct results out of the applicability range of independent reference theory.

IV. ON THE FITTING TO NUMERICAL CALCULATIONS

As an independent reference theory in their earlier work, WMS used the numerical calculation in the frame of standard Luttinger model. WMS chose the functional dependence of the cutoff parameter $q_0$ and correlation functions by fitting to the numerical results. For this purpose, the standard expressions for the correlation functions of the Luttinger model with short-ranged interaction were modified by introducing fitting parameters in the exponents.

The shortcomings of such approach are evident. First, correlation functions are of primary interest in the threshold region, where they either diverge or quickly go to zero; however, it is in these regions that the accuracy of numerical calculations is least trustworthy. Second, the fitting formulas do not follow from any physical theory, but rather represent a formal mathematical interpolation.

Moreover, one has serious grounds to doubt whether WMS’s fitting to numerical calculations is valid.

1) The formula for the electron Green function used in WMS’s calculations is incorrect. Specifically, Eqs. (4), (5) of Ref. 1 contradict to the very definition of the Green function. Green’s function is defined as $G_0 \equiv \langle \psi_r(x,t)\psi_r^\dagger(0,0) \rangle$, where $r$ refers to the right-moving ($r = +1$) or left-moving ($r = -1$) particles. The Fourier-transform of the Green function $G_r(q, \omega)$ possesses the fundamental property: at zero temperature, $G_r(q, \omega) = 0$ if $\omega < 0$, the energy $\omega$ being measured from the chemical potential $\mu$. WMS’s results (4), (5) show that the Green function of the left-moving particles $G_{r=1}(x, t)$ is analytic in the upper half-plane of the complex variable $\omega$. This immediately gives that Green’s function $G_{r=-1}(q, \omega) \neq 0$ at $\omega < 0$, but instead $G_{r=-1}(q, \omega) = 0$ at $\omega > 0$. Thus analytic and spectral properties of the electron Green function are violated in WMS’s work.

2) Fitting procedure uses the behavior of the spectral function $\rho(q, \omega)$ at frequencies much larger then the Fermi energy, where the Luttinger model is not justified. Thus, they introduce some ‘previously overlooked energy scale’ $\omega_s$ that is defined as $\omega_s = 50(v_F/d)\sqrt{V_0}\exp(1/V_0)$, with $V_0 = 4e^2/\pi v_F$ being a dimensionless measure of the interaction strength. The spectral function is considered at $\omega > \omega_s$. Note that $\omega_s$ is of several orders of magnitude greater than the electron Fermi energy, which is far beyond the scope of the exploited approach!

3) The expression for the quasi-1D Coulomb interaction potential is incorrect in the high-momentum region,
that the velocity translation functions of the Coulomb Luttinger liquid in the

to determine the exact behavior of the dynamic corre-

with the short-range cutoff $\Lambda \approx 2.5/d$, $d$ being the diam-

er of the quantum wire, see Eq. (2) of Ref. 4. WMS denote the short-range cutoff also by $q_0$, but here we re-

serve $q_0$ for the long-range cutoff. WMS claim that the potential should be $1/q$ for $q$ larger than some scale $\Lambda$ set by the geometry and the wave function size. Eq. (16) indeed guarantees that.

However, such behavior is incorrect, since the potential should behave as $1/q^2$ in the high-momentum region. The correct formula is derived in Appendix A,

$$V(q) = 2e^2 \ln \left[ \frac{\Lambda^2 + q^2}{q^2} \right] , \quad (15)$$

It describes adequately the behavior of the quasi-1D Coulomb potential both in the long-wave ($V(q) \approx 2e^2 \ln q d$) and in the short-range ($V(q) \approx e^2 \Lambda^2/q^2$) regions.

Generally, WMS uncritically overestimate their results pertaining to the region of high $q$ and $\omega$.

Thus, using Eq. (15), WMS found the strange behavior of the plasmon frequency $\omega_q$ at $q \gg d^{-1}$, namely $\omega_q \sim q v_F + \text{const.}$ This is not a unique property of CLL, as they assert, but a trivial mistake. Correct Eq. (16) gives $\omega_q \sim q v_F$, without any additional constant.

They also discovered some dramatic modifications of $\rho(q, \omega)$ at $\omega \gg \omega_s$ as compared to the short-ranged interaction case due to the slow ($1/q$) decay of the Coulomb interaction in the large momentum region. The passion fades if one remembers that Eq. (16) for Coulomb potential is incorrect, and bosonization does not work there.

$$\rho(q, \omega) = \frac{v_F}{4\omega} \int_0^{\infty} dQ \frac{1}{q} \left( 1 - \operatorname{sign} \frac{q}{g(q)} \right)^2 \rho(Q, \omega - \omega_q) + \ldots \quad (18)$$

In the case of Coulomb interaction, it is sufficient to consider only the first term of the expansion in the RHS of Eq. (18) to obtain the correct asymptotic behavior of $\rho(q, \omega)$ at $\delta \to 0$.

On the RHS of Eq. (18), the integral $\int_0^{\infty} dQ \rho(Q, \omega - \omega_q)$ equals, up to a factor, the tunnelling density of states $N(\omega - \omega_q)$, which has a soft gap in the Coulomb interaction case. Consequently, our method shows that the spectral function $\rho(q, \omega)$ turns to zero as $\omega \to \omega_q$, i.e. it contains a pseudogap. The functional dependence of the tunnelling density of states can be obtain either via direct integration, or, more elegantly, by solving the integral equation, similar to (17).

Finally, in the limit $\delta \to 0$ we obtain

$$\rho(q, \omega) \sim \frac{A(q)}{\omega} |\ln \delta|^{1/2} \exp \left[ -\frac{1}{3\beta} |\ln \delta|^3 \right] , \quad (19)$$

where $A(q) = \left[ 1 - g^{-1}(q) \right]^2$. The obtained form of the spectral function is consistent with numerical and experimental results, without any mystique.

VI. CONCLUSION

To summarize, our theory describes exactly the threshold behavior of the CLL correlators. In contrast, the 'effective exponent theory' strongly distorts the interaction, making it neither short-ranged nor Coulomb one. This is the main reason of the discrepancy between our results.

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APPENDIX A: QUASI-ONE-DIMENSIONAL COULOMB INTERACTION POTENTIAL

Here we derive the interaction potential of electrons, confined in a 1D quantum wire and interacting via Coulomb long-ranged forces. The pair interaction potential equals

$$U(x_1, x_2) = e^2 \int G(r_1 - r_2) \rho(r_{1\perp}) \rho(r_{2\perp}) dx_{1\perp} dx_{2\perp}.$$  \hspace{1cm} (A1)

The $x$-axis is directed along the wire, $r_i \equiv (x_i, y_i, z_i)$, $r_{i\perp} \equiv (y_i, z_i)$. $\rho(r_{\perp})$ is the transverse density distribution in the wire, with only first subband populated. The transverse distribution is supposed to be localized on scale of $r_\perp \approx d$. The Green function is

$$G(r) = \frac{1}{|r|}, \quad G(k) = \frac{4\pi}{k^2}. \hspace{1cm} (A2)$$

Denote $x = x_1 - x_2$. The long-distance ($x \to \infty$) behavior of the potential can be well approximated by $U(x) \approx e^2/\sqrt{x^2 + d^2}$. Although this simple approximation leads to correct logarithmic behavior of the Fourier-transformed potential in the long-wave region of $q \to 0$, it is insufficient to obtain correct expression in the short-range region. Below one finds a general derivation.

Represent the Green function in Eq. (A1) via the Fourier integral to get

$$U(q) = e^2 \int \frac{dk_\perp}{2\pi^2 k^2} e^{iqr} e^{-ik(r_1 - r_2)} \rho(r_{1\perp}) \rho(r_{2\perp}) dx_{1\perp} dx_{2\perp}. \hspace{1cm} (A3)$$

Performing integration w.r.t. $x$ gives $\delta$-function, which eliminates integration w.r.t. $k_x$. Integration w.r.t. $r_{i\perp}$ yields

$$U(q) = e^2 \int \frac{dk_\perp}{\pi} \frac{1}{q^2 + k_{\perp}^2} |\rho(k_{\perp})|^2. \hspace{1cm} (A4)$$

For cylindric wire this becomes

$$U(q) = e^2 \int 0^\infty 2kdk \frac{1}{q^2 + k^2} |\rho(k)|^2. \hspace{1cm} (A5)$$

Use the fact that $\rho(k)$ has a scale $A \approx 1/d$, such that $\rho(k)$ is small at $k > A$. Neglecting for simplicity the $k$-dependence of $\rho(k)$ for $0 < k < A$, one gets

$$U(q) = e^2 \int 0^A 2kdk \frac{1}{q^2 + k^2} = e^2 \ln \left[ \frac{A^2 + q^2}{q^2} \right]. \hspace{1cm} (A6)$$

At $qd \ll 1$, this gives the logarithmic divergency

$$U(q) \approx 2e^2 \ln \left[ \frac{1}{qd} \right]. \hspace{1cm} (A7)$$

When $qd \gg 1$,

$$U(q) \approx e^2 \frac{A^2}{q^2}. \hspace{1cm} (A8)$$

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