New sum rules relating the 1-body momentum distribution of the homogeneous electron gas to the Overhauser 2-body wave functions of its pair density

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(Dated: November 15, 2018)

The recently derived sum rules for the scattering phase shifts of the Overhauser geminals (being 2-body-wave functions which parametrize the pair density together with an appropriately chosen occupancy) are generalized to integral equations which allow in principle to calculate the momentum distribution, supposed the phase shifts of the Overhauser geminals are known from an effective parity-dependent interaction potential (screened Coulomb repulsion).

PACS numbers: 71.10.Ca,05.30.Fk,71.15.Mb

Keywords: electron gas, two-body reduced density matrix, contraction sum rule
Introduction

The homogeneous electron gas is a model which allows to study pure electron correlation without any interference with the multiple-scattering problem of real molecules, clusters, and solids. The quantum kinematics of this phenomenon is hidden in the reduced density matrices and their diagonals. The simplest reduced densities are (only the spin-unpolarized ground state is considered here) the 1-body momentum distribution \( n(k) \), recently parametrized in terms of the convex Kulik function, and the 2-body quantities \( g_{\uparrow\uparrow}(r) \) and \( g_{\uparrow\downarrow}(r) \), being the non-negative pair densities (PDs) for electron pairs with parallel respectively antiparallel spins and with an interelectronic distance \( r \). All these quantities depend parametrically on the electron density \( \rho(3/(4\pi r_s^3)) \). Correlation induced properties of \( n(k) \) (normalized as \( (2/N) \sum_k n(k) = 1 \)) are: (i) its nonidempotency \( 0 < n(k) < 1 \), measured by a quantity \( c = (2/N) \sum_k n(k)[1-n(k)] < 1 \) (which is christened here Löwdin parameter [12]) and (ii) the quasi-particle weight \( z_F = n(1^-) - n(1^+) < 1 \) (\( k \) is measured in units of the Fermi wave length \( 1/(\alpha r_s) \), \( \alpha = (4/9\pi)^{1/3} \)). Correlation induced properties of the PDs with their asymptotics \( g_{\uparrow\uparrow}(\infty) = 1 \) are besides the oscillatory behavior for \( r \to \infty \), for small \( r \) the Fermi hole \( g_{\uparrow\uparrow}(r) < 1 \) with its on-top properties \( g_{\uparrow\uparrow}(0) = 0 \), \( g_{\uparrow\downarrow}'(0) = 0 \), and a characteristic curvature \( g_{\uparrow\downarrow}''(0) > 0 \) and the Coulomb hole \( g_{\uparrow\downarrow}(r) < 1 \) with its characteristic on-top value \( g_{\uparrow\downarrow}(0) < 1 \). The on-top curvature of the Fermi hole is a local measure of the correlation strength. With the spin-summed PD \( g = [g_{\uparrow\uparrow} + g_{\uparrow\downarrow}]/2 \), particle-number fluctuations in spatial parts (fragments, domains) of the system can be discussed as another correlation index with the conclusion "correlation suppresses fluctuations". For the ideal Fermi gas \( (r_s = 0) \) it is \( n^{(0)}(k) = 1 - \Theta(k) \), \( c^{(0)} = 0 \), \( z_F^{(0)} = 1 \), and \( g_{\uparrow\downarrow}^{(0)}(r) = 1 \).

The virial theorem [25] provides a relation between the kinetic and the interaction energy, which follow from \( n(k) \) and \( g(r) \), respectively, giving thus for their \( r_s \) dependence an integral relation. In this paper another relation between \( n(k) \) and \( g(r) \) is derived. This derivation is based on the successful parametrization of the PDs in terms of Overhauser 2-body wave functions (geminals), which are the scattering state solutions of an effective 2-body Schrödinger equation with an appropriately screened Coulomb repulsion. It is furthermore based on the assumption that these Overhauser geminals can be used to represent also the 2-body reduced density matrix (2-matrix) \( \gamma_2(1|1', 2|2') \), the digonal of
which gives the PD. Now the idea was to obtain the 1-matrix $\gamma_1$ from the contraction of the 2-matrix $\gamma_2$. Unfortunately for extended systems this does not work, because this contraction is not size-extensive. This problem is easy to overcome with the help of the cumulant expansion. \[20, 32, 33, 34, 35\] It defines by $\gamma_2 = A\gamma_1\gamma_1 - \chi$ ($A = \text{antisymmetrizer}$) the size-extensively normalizable and contractable cumulant 2-matrix $\chi = A\gamma_1\gamma_1 - \gamma_2$, which is here thus represented in terms of Bessel functions (from $A\gamma_1\gamma_1$) and Overhauser geminals (from $\gamma_2$). From the normalization of $\chi$ follow sum rules (SRs) for the scattering phase shifts of the Overhauser geminals. [31] These (Friedel like) SRs are generalized in this paper by using the contraction properties of $\chi$, such that (at least in principle) $n(k)$ can be calculated supposed the phase shifts of the Overhauser geminals are known.

### Basic notation and normalization sum rules

The singlet (+ for even $l$)/triplet (− for odd $l$) components of the PD in terms of Overhauser geminals $R_l(r, k)$ are

$$g_\pm(r) = \sum_L \chi_\pm^L < \mu(k)R_l^2(r, k) >, \quad L = (l, m_l).$$

The $k$-average is defined by

$$< \cdots > = \frac{2}{N} \sum_k \cdots = \frac{2}{N} \int_0^\infty \frac{\Omega d^3 k}{(2\pi)^3} \cdots = \int_0^\infty d(k^3) \cdots$$

with the normalization volume $\Omega$ and the density $\varrho = N/\Omega = 1/3\pi^2$. Wave lengths are measured in units of the Fermi wave length $k_F = 1/(\alpha r_s)$, $\alpha = (4/(9\pi))^{1/3}$. In this paper the Overhauser occupancy is slightly generalized by

$$\mu(k) = \frac{2}{N} \sum_K \mu(K, k), \quad \mu(K, k) = n(|\frac{1}{2}K + k|)n(|\frac{1}{2}K - k|),$$

because it arises here not from the idempotent $n^{(0)}(k) = \Theta(1 - k)$ of the ideal Fermi gas, but from the nonidempotent $n(k)$ of the interacting electron gas. [7, 8] It is $\mu(0) = 8(1 - c)$. The $R_L(r, k) = R_l(r, k)Y_L(e_r)$ are the (scattering state) solutions of the 2-body Schrödinger equation (the center-of-mass motion separates completely)

$$[-\Delta + v_\pm(r) - k^2]R_L(r, k) = 0, \quad v_\pm(\infty) = 0$$

with an appropriate repulsive interaction potential $v_\pm(r) = 2\alpha r + \cdots$, possibly different for “+” or “−”. [27, 28, 29, 30, 31] The success of the Overhauser approach means, that
local interaction potentials \( v_+ (r) \) and \( v_- (r) \), if not being exact, are at least reasonable approximations.

One generalization of Eq.(1) concerns inhomogeneous systems. Here another generalization is considered, namely the representation of the 2-matrix in terms of Overhauser geminals:

\[
\gamma_\pm (R|R', r|r') = \varrho^2 (4\pi)^2 \sum_{L,L'}^{\pm} < \tilde{\mu}_{LL'} (R - R', k) R_L (r, k) R_{L'} (r', k) >
\]

\( R = \frac{1}{2} (r_1 + r_2) \) is the center-of-mass coordinate and \( r = r_1 - r_2 \) is the relative coordinate. As \( \mu(k) \), the \( l \)-independent but \( k \)-dependent weight in Eq.(1), also here the occupancy matrix

\[
\tilde{\mu}_{LL'} (R, k) = \frac{2}{N} \sum_K e^{iKR} \mu_{LL'} (K, k) = \int \frac{d\Omega_k}{4\pi} Y_L^* (e_k) \mu (K, k) Y_{L'} (e_k)
\]

follows with Eq. (3) from the momentum distribution \( n_k \).

Arguments in favour of Eq.(5) are: (i) The diagonal elements give the Overhauser PD Eq.(1), \( \gamma_0 (R|R, r|r) = \varrho^2 g_\pm (r) \), and (ii) in the cumulant partitioning of \( \gamma_\pm \) the generalized HF term \( \gamma_{HF}^\pm \) is given by the same expression as Eq.(5) with only \( R_L (r, k) \) replaced by \( j_L ( kr) \) because the natural orbital are plane waves and using the \( L \)-expansion of a plane wave, \( \exp (i kr) = 4\pi \sum_L i^L j_L (kr) Y_L^* (e_k) \).

So the cumulant 2-matrix \( \chi_\pm = - (\gamma_\pm - \gamma_{HF}^\pm) \) is given by

\[
\chi_\pm (R|R', r|r') = - \varrho^2 (4\pi)^2 \sum_{L,L'}^{\pm} < \tilde{\mu}_{LL'} (R - R', k) [R_L (r, k) R_{L'} (r', k) - j_L (kr) j_{L'} (kr')] >
\]

For the normalization

\[
\int d^3r \ \chi_\pm (R|R, r|r) = - \varrho^2 \int d^3r \sum_L^{\pm} < \mu(k) [R^2_l (r, k) - j^2_l (kr)] > = \varrho \sum_L^{\pm} \int_0^\infty dk \mu(k) n^l_k (k) = \pm \varrho c,
\]

cf. Ref. [31].

**Contraction sum rules**

With the contracted cumulant 2-matrices and their Fourier transform

\[
\chi_\pm (|r_1 - r'_1|) = \int d^3r_2 \chi_\pm (R|R', r|r') \bigg|_{r_2 = r_2}, \quad \bar{\chi}_\pm (k) = \frac{1}{2} \varrho \int d^3r \ e^{-ikr} \chi_\pm (r),
\]
the contraction SRs are
\[ \tilde{\chi}_\pm(\kappa) = \mp e n(\kappa)[1 - n(\kappa)]. \] (10)

They follow from \( \tilde{\gamma}_\pm(\kappa) = e n(\kappa)[\frac{1}{2} N \pm 1], \tilde{\gamma}_{HF}^H(\kappa) = e n(\kappa)[\frac{1}{2} N \pm n(\kappa)], \) and \( \tilde{\chi}_\pm = \tilde{\gamma}_\pm^H - \tilde{\gamma}_\pm, \)

showing explicitly the cancellation of the non-size extensive terms. Eq. (10) says that \( n(k) \)
can be calculated, if the lhs is known. With \( \chi_\pm(0) = \frac{2}{N} \sum_\kappa \tilde{\chi}_\pm(\kappa) = \mp e c \) the special phase
shift SRs of Ref. [31] are contained in the more general SRs (10) as special cases.

With the identity (following from Eq. (4) and generalizing Eq. (13) of Ref. [31])
\[ R^*_L R_L' = \left( \frac{\partial}{\partial r} + \frac{\partial}{\partial r'} \right) \frac{1}{2} \left[ \frac{\partial R^*_L}{\partial r} \frac{\partial R_L'}{\partial r'} - R_L \frac{\partial R^*_L}{\partial r'} + \text{h.c.} \right] \]
\[ - \frac{1}{2} [v_\pm(r) - v_\pm(r')] \left[ R_L R_L' - R_L R_L' \right], \] (11)

(where \( R^*_L = R_L(r', k), \dot{R}_L = \partial R_L(r, k)/\partial k^2, \) and h.c. means complex conjugate together
with an exchange in both coordinates and indices) from Eqs. (8) and (9) it turns out
\[ \chi_\pm(r) = \chi^A_\pm(r) + \chi^B_\pm(r) = -e^2 4\pi \sum_{L,L'}^{\pm} \left( \frac{1}{2} r, k \right) \left[ A_{LL'}(r, k) + B_{LL'}(r, k) \right] . \] (12)
The A and B matrices are defined by
\[ A_{LL'}(r, k) + B_{LL'}(r, k) = 4\pi \int_{r' < R \to \infty} d^3r' \left[ R_L(r + r', k) R_{L'}^*(r', k) - j_L(k(r + r')) j_{L'}^*(kr') \right] \] (13)
where \( A_{LL'} \) results from the 1st term of Eq. (11) and \( B_{LL'} \) from the 2nd one. With the Gauss
theorem it is
\[ A_{LL'}(r, k) = \delta_{LL'} 4\pi R^2 \left[ \frac{\partial R^*_L}{\partial R} \dot{R}_L - \dot{R}_L \frac{\partial \dot{R}_L}{\partial R} - \frac{\partial j_L}{\partial R} \dot{R}_L + j_L \frac{\partial \dot{R}_L}{\partial R} \dot{R}_L \right]_{R \to \infty}, \] (14)

(where \( R_L = R_L(R, k) \) and the \( r \)-dependence disappears) and with the analysis of Ref. [31]

it is finally
\[ A_{LL'}(r, k) = \delta_{LL'} A_l(k), \quad A_l(k) = \frac{2\pi}{k^2} \phi_l(k) . \] (15)

So
\[ \chi^A_\pm(r) = -e^2 \sum_{L}^{\pm} \frac{2}{N} \sum_{K} e^{iK \cdot r} < \mu(K, k) A_l(k) >, \quad \mu(K, k) = \int \frac{d\Omega_k}{4\pi} \mu(K, k). \] (16)

Because of \( \chi^B_\pm(0) = 0 \) and Eq. (3), it results \( \chi_\pm(0) = -e^2 \sum_L^{\pm} < \mu(k) A_l(k) >, \) in agreement with the (Friedel like) phase shift SRs of Ref. [31], saying \( \chi_\pm(0) = \mp e c. \) The Fourier transform
\[ \tilde{\chi}^A_\pm(\kappa) = -e^2 \sum_L^{\pm} < 2^3 \mu(2\kappa, k) A_l(k) >, \] (17)
enters (together with the \( B \) term) the more general SR (14).

As already mentioned, the \( B \) matrix of Eq. (13) follows from the 2nd term of Eq. (11)

\[
B_{LL'}(\mathbf{r}, k) = -4\pi \int d^3 r' \frac{1}{2} [v_\pm(|\mathbf{r} + \mathbf{r}'|) - v_\pm(\mathbf{r}')] \times \\
\left[ R_L(\mathbf{r} + \mathbf{r}', k) \left( R^*_L(\mathbf{r}', k) - \tilde{R}_L(\mathbf{r} + \mathbf{r}', k) \tilde{R}^*_L(\mathbf{r}', k) \right) \right]. \tag{18}
\]

So

\[
\chi^B_\pm(\mathbf{r}) = -\theta^2 4\pi \sum_{L,L'}^{\pm} < \tilde{\mu}_{LL'} \left( \frac{1}{2} \mathbf{r}, k \right) B_{LL'}(\mathbf{r}, k) > \tag{19}
\]

and

\[
\tilde{\chi}^B_\pm(\kappa) = -\frac{1}{2} \theta^2 4\pi \sum_{L,L'}^{\pm} < \tilde{\mu}_{LL'}(2(\kappa - \kappa_1), k) \tilde{B}_{LL'}(\kappa_1, k) > . \tag{20}
\]

Note \( \sum_\kappa \tilde{\chi}^B_\pm(\kappa) = 0 \). Thus the \( B \) term does not contribute to the normalization of \( n(k) \) as it does not contribute to the normalization of the PDs.

The Fourier transformed interaction potential and Overhauser geminals

\[
\tilde{v}_\pm(\kappa) = \theta \int d^3 r e^{-i\kappa \mathbf{r}} v_\pm(\mathbf{r}), \quad \tilde{R}_L(\kappa, k) = \theta \int d^3 r e^{-i\kappa \mathbf{r}} R_L(\mathbf{r}, k) \tag{21}
\]

determine the Fourier transformed \( B \) matrix

\[
\tilde{B}_{LL'}(\kappa_1, k) = -\frac{4\pi}{2} \frac{2}{4\theta N} \sum_{\kappa_2} \tilde{v}_{\pm}(\kappa_{12}) \left[ \tilde{R}_L(\kappa_2, k) \tilde{R}^*_L(\kappa_1, k) - \tilde{R}_L(\kappa_1, k) \tilde{R}^*_L(\kappa_2, k) \right], \tag{22}
\]

\( \kappa_{12} = |\kappa_1 - \kappa_2| \). Eq. (22) has to be inserted into Eq. (20). Then with \( (\zeta_{12} = \mathbf{e}_1 \mathbf{e}_2) \)

\[
v_{\pm}(\kappa_{12}) = \sum_{L', L''} P_{L''}(\zeta_{12}) v^\pm_{L''}(\kappa_1, \kappa_2) \quad \text{or} \quad v^\pm_{L''}(\kappa_1, \kappa_2) = \int_{-1}^{1} \frac{d\zeta_{12}}{2} P_{L''}(\zeta_{12}) v_{\pm}(\kappa_{12}) \tag{23}
\]

and with

\[
\int \frac{d\Omega_\kappa}{4\pi} \mu(2(\kappa - \kappa_1), k) = \sum_{L_1} P_{L_1}(\mathbf{e}_1 \mathbf{e}_k) \mu_{L_1}(\kappa, \kappa_1, k) \tag{24}
\]

(the invariance of \( \mu(\mathbf{K}, \mathbf{k}) \) by the replacement \( \mathbf{k} \rightarrow -\mathbf{k} \) makes \( l_1 \) even) and with

\[
C_{ll_1 l'} = \int d\Omega P_l(\zeta) P_{l_1}(\zeta) P_{l'}(\zeta) \tag{25}
\]

(because \( l \) and \( l' \) have the same parity, these coefficients vanish for odd \( l_1 \)) an expression arises,

\[
\tilde{\chi}^B_{\pm}(\kappa) = \theta \sum_{L,L'}^{\pm} \sum_{L_1} C_{ll_1 l'} \left( \frac{2}{N} \right)^2 \sum_{\kappa_{1,2}} < \mu_{l_1}(\kappa, \kappa_1, k) \times \\
\left[ v^\pm_{L_1}(\kappa_1, \kappa_2) \tilde{R}_L(\kappa_2, k) \tilde{R}^*_L(\kappa_1, k) - \tilde{R}_L(\kappa_1, k) \tilde{R}^*_L(\kappa_2, k) v^\pm_{L_1}(\kappa_2, \kappa_1) \right] >, \tag{26}
\]
which vanishes, because the $L-L'$ double sum runs over an antisymmetric matrix (each element $l, l'$ is compensated by its mirror party). Thus, it finally results
\[
\frac{2}{\pi} \sum_{L}^{\pm} < \frac{2^3 \mu(2\kappa, k)}{3k^2} \eta_l^\prime(k) > = \pm n(k)[1 - n(k)]. \tag{27}
\]

The occupancy weight in Eq. (27) can be written in terms of $n(k)$ as
\[
\mu(2\kappa, k) = \int \frac{d\Omega_k}{4\pi} n(|\kappa + k|)n(|\kappa - k|), \tag{28}
\]
or with $n(k) = \frac{1}{2} \rho \int d^3 r \frac{\sin \kappa r}{\kappa r} f(r)$ in terms of the dimensionless 1-matrix $f(r)$ as
\[
\mu(2\kappa, k) = \frac{1}{4\rho^2} \int d^3 r_1 d^3 r_2 \frac{\sin \kappa |r_1 + r_2|}{\kappa |r_1 + r_2|} \frac{\sin k |r_1 - r_2|}{k |r_1 - r_2|} f(r_1)f(r_2). \tag{29}
\]

For the momentum distribution the parametrization in terms of the Kulik function can be used. [7, 8]

Conclusions

The contraction SRs (27) are nonlinear integral equations for $n(k)$ supposed the phase shifts of the Overhauser geminals $R_l(r, k)$ are known from the effective interaction potential $v_\pm(r) = \frac{ar^a}{r} + \cdots$. These integral equations have to be solved selfconsistently. Because the PD is (via the $R_l(r, k)$) a functional of $v_\pm(r)$ and $n(k)$ is a functional of the $R_l(r, k)$, thus the total energy becomes a functional of $v_\pm(r)$.

The success of the Overhauser approach seems to confirm the possibility of a pair-density functional theory, the idea of which is presented in Ref. [36]. Whereas therein the geminal occupancy was erroneously assumed to be 1 and 0 according to occupied and unoccupied geminals respectively (analog to the aufbau principle of the Hartree-Fock and the Kohn-Sham schemes), in the Overhauser approach a geminal occupancy $\mu(k)$ is used being quite different from a step function. For PD or 2-matrix geminals there is no aufbau principle.

Acknowledgments

One of the authors (P.Z.) gratefully acknowledges J.P. Perdew, P. Gori-Giorgi, and M.P. Tosi for inspiring discussions and P. Fulde for supporting this work. Another author (K.P.)
expresses her thanks to the Max Planck Institute for the Physics of Complex Systems for hospitality and F.T. thanks H. Eschrig for his support of this work and Technische Universität Dresden for a scholarship.

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