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Screening in quantum charged systems

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For stationary states of quantum charged systems in ν dimensions, $\nu \geq 2$, it is proven that the reduced-density matrices satisfy a set of sum rules whenever the clustering is faster than $|x|^{-(\nu+l)}$. These sum rules, describing the screening properties, are analogous to those previously derived for classical systems. For neutral quantum fluids, it is shown that the clustering cannot be faster than the decay of the force.

I. INTRODUCTION

In this paper, we generalize to quantum systems the sum rules which have been obtained for classical charged systems.[1-3] In the classical case we proved that if the correlations cluster faster than $|x|^{-(\nu+l)}$ (ν is the space dimensionality), then the l first multipole moments of the charge density, $l=0,1,2,\ldots,$ induced by specifying the position of any n particles must vanish. This implied a number of exact sum rules, the first one (corresponding to $l=0$) being the well-known electroneutrality condition. We show here that under the same clustering assumptions the diagonal part of the reduced density matrices (RDM) obey the same relations. Moreover the off-diagonal part of the RDM satisfy a similar set of sum rules which are specific to the quantum-mechanical situation. This holds for systems with several kinds of particles having arbitrary statistics.

As in the classical case, the origin of the sum rules lies in the long range of the Coulomb force. Generally, the sum rules will hold whenever the rate of clustering of the correlations is faster than the decay of the potential. Since charged systems are expected to have good clustering properties at sufficiently high temperature (Debye screening has been proved rigorously in the classical case[4,5]) the sum rules will be true in such phases. As a consequence, their implication on the nature of the fluctuations developed in Refs. 6 and 7 can be directly carried over the quantum-mechanical description. In particular, the bulk charge fluctuations are of the order of the surface,[6] the covariance of the potential and the field can be expressed in terms of the diagonal part of the RDM and have slowly decaying parts as in Ref. 7. Other applications will be discussed elsewhere.[8]

Our study of the quantum situation is analogous to the classical one. We consider stationary states of infinite charged systems described locally in terms of reduced density matrices (recall that the existence of the RDM has been established for short-range interactions at high temperatures and small activities,[9] and for systems of two types of charged bosons with same masses, activities and opposite charges[10]). These RDM are assumed to satisfy the usual Bogoliubov hierarchy of equations expressing the stationarity of the state.[11] The sum rules follow then from an analysis of the asymptotic behavior of these equations as one of the particles is sent to infinity. It is worth noting that in this derivation the equilibrium conditions are not used but only the stationarity and some invariance properties of the state. In particular the sum rule will hold for equilibrium states having sufficiently fast clustering properties.

In Sec. II, we give the general quantum-mechanical setting and the sum rules are derived in Sec. III. Some generalizations are considered in Sec. IV. As an application it is shown that the correlations of a quantum fluid with infinite range but integrable potential (e.g., Lenard-Jones interactions) cannot decay faster than the force. For the sake of convenience, we state in the Appendix two lemmas of Ref. 2 which we use in the asymptotic analysis.

II. GENERAL SETTING

The system consists of N species of quantum particles with mass m_α, charge e_α, chemical potential μ_α, and statistics ϵ_α, $\alpha=1,\ldots,N$ ($\epsilon=+1$ for bosons and $\epsilon=-1$ for fermions). The particles move in the whole ν-dimensional space $\mathbf{R}^\nu$ and interact by means of the Coulomb potential

$$\phi^{(c)}_{\alpha_1\alpha_2}(x_1-x_2)=e_{\alpha_1}e_{\alpha_2}\begin{cases}\dfrac{1}{|x_1-x_2|^{\nu-2}} & \text{if } \nu\neq 2\\ -\ln|x_1-x_2| & \text{if } \nu=2\end{cases}. \tag{2.1}$$

The particles may be submitted to the action of static external forces such as the field due to a fixed distribution of charges, or forces which are not of electrical nature (walls).

In order to emphasize the special properties due to the long range of the potential and to take into account additional short-range interactions, we shall consider a more general class of translation invariant two-body potentials $\phi_{\alpha_1\alpha_2}(x_1,x_2)$ with a power-law decay at infinity; we assume that $\phi_{\alpha_1\alpha_2}(x_1,x_2)$ satisfies the following conditions:

(1) $\phi_{\alpha_1\alpha_2}(x_1-x_2)=e_{\alpha_1}e_{\alpha_2}\phi(|x_1-x_2|)$,

(2) $\phi(x)$ is locally integrable, twice differentiable and

$$\lim_{\lambda\to\infty} \lambda^{\gamma}\phi(\lambda\hat{u})=d_0\neq 0,\quad |\hat{u}|=1$$

$$\lim_{\lambda\to\infty} \lambda^{\gamma+1}(\partial_i\phi)(\lambda\hat{u})=d_1\hat{u}_i,\quad d_1\neq 0$$

$$\partial_{ij}\phi(x)=o\left[\frac{1}{|x|^{\gamma+1}}\right] \text{ as } |x|\to\infty .$$

The case $\gamma=\nu-2$ corresponds to a potential which is asymptotically like the Coulomb potential. The case $\gamma>\nu$ and $\alpha=1$ corresponds to a quantum fluid with one kind of particle interacting with an infinite range integrable potential. If the particles have spins, α will label the species of the particle together with its spin state, and our whole discussion applies provided that the potential is spin independent.

The state of the system is described by the *reduced density matrices* $\rho(Q\mid Q')$, formally defined as

$$\rho(Q\mid Q')=\rho(q_1,\ldots,q_k\mid q_1',\ldots,q_l') =\langle a^*(q_1')\cdots a^*(q_l')a(q_k)\cdots a(q_1)\rangle , \tag{2.2}$$

where Q and Q' are the ordered sets

$$Q=(q_1,\ldots,q_k),\quad Q'=(q_1',\ldots,q_l'),\quad |Q|=k ,$$
$$|Q'|=l,\quad q=(x,\alpha),\quad x\in\mathbb{R}^\nu,\quad \alpha=1,2,\ldots,N .$$

The creation and annihilation operators $a^*(q),a(q)$ satisfy the canonical commutation relations

$$[a(x,\alpha),a^*(y,\alpha)]_{-\epsilon_\alpha}=\delta(x-y) ,$$
$$[a(x,\alpha),a(y,\alpha)]_{-\epsilon_\alpha}=0 ,$$
$$[a(x,\alpha),a^*(y,\beta)]_-=[a(x,\alpha),a(y,\beta)]_-=0 \quad \text{if } \alpha\neq\beta .$$

From these relations and the formal representation (2.2) one can easily infer the symmetry properties of $\rho(Q\mid Q')$; in particular the RDM are Hermitian, i.e., $\rho(Q\mid Q')^*=\rho(Q'\mid Q)$. In the following we shall use the notation $\delta_{q_1q_2}=\delta_{\alpha_1\alpha_2}\delta(x_1-x_2)$ and

$$\int dq=\int_{\mathbb{R}^\nu} dx\sum_\alpha .$$

By definition the state is *gauge invariant* (with respect to the charge) if

$$(C(Q)-C(Q'))\rho(Q\mid Q')=0 \quad\text{for all } Q,Q'$$

where

$$C(Q)=\sum_{i=1}^{k} e_{\alpha_i} . \tag{2.3}$$

The state is *invariant under time reversal* if

$$\rho(Q\mid Q')=\rho(Q'\mid Q) \quad\text{for all } Q,Q' \tag{2.4}$$

i.e., the density matrices are real.

The state is *translation invariant* if

$$\rho(Q+a\mid Q'+a)=\rho(Q\mid Q') , \tag{2.5}$$

where

$$Q+a=((x_1+a,\alpha_1),\ldots,(x_k+a,\alpha_k))$$

and similar relations for the invariance under rotations and space reflection.

Throughout the whole paper we are concerned with "stationary states" (i.e., invariant under the time evolution). The RDM are then solution of the following Bogoliubov hierarchy (see Ref. 11):

$$-(H(Q)-H(Q'))\rho(Q\mid Q')=\int dq\left[\sum_{i=1}^{k}\phi(q_i,q)-\sum_{j=1}^{l}\phi(q_j',q)\right][\rho(Q,q\mid Q',q)-\rho(Q\mid Q')\rho(q\mid q)] , \tag{2.6}$$

where

$$H(Q)=\sum_{i=1}^{k}\left[-\frac{\hbar^2}{2m_{\alpha_i}}\Delta_{x_i}+\mu_{\alpha_i}+\phi_\rho(q_i)\right] +\sum_{\substack{i,j=1\\ i<j}}^{k}\phi(q_i,q_j)$$

is the $|Q|$-particle Hamiltonian; Δ_x is the Laplacian acting on the coordinates of the α particle; and $\phi_\rho(q)$ is the total average potential on species α at x.

This potential $\phi_\rho(q)$ has a short-range contribution $\phi_\rho^{(s)}(q)$ and a Coulomb contribution $\phi_\rho^{(c)}(q)$, i.e.,

$$\phi_\rho(q)=\phi_\rho^{(s)}(q)+\phi_\rho^{(C)}(q) ,$$
$$\phi_\rho^{(s)}(q)=\phi^{\text{ext}(s)}(q)+\int dq_1\phi^{(s)}(q,q_1)\rho(q,q_1) ,$$

$\phi^{\text{ext}(s)}(q)$ and $\phi^{(s)}(q,q_1)=\phi(q,q_1)-\phi^{(C)}(q,q_1)$ are the non-Coulombic part of the potentials, and $\phi_\rho^{(C)}(q)=e_\alpha\phi_\rho^{(C)}(x)$, where $\phi_\rho^{(C)}(x)$ is solution of

$$\Delta\phi_\rho^{(C)}(q)=\omega_\nu C_\rho(x)\ (\omega_1=2,\ \omega_2=2\pi,\ \omega_3=4\pi)$$

with

$$C_\rho(x)=\sum_\alpha e_\alpha\rho(x,\alpha;x,\alpha)+C^{\text{ext}}(x)$$

the total charge density at x. This formulation of the Bogoliubov equation for Coulomb systems is analogous to the classical one.[2]

We assume that the RDM have the following clustering properties as one particle is sent to infinity:

$$\rho(Q,q\mid Q',q')-\rho(q\mid q')\rho(Q\mid Q')=O\left[\frac{1}{|x|^\eta}\right] \tag{2.7}$$

with $q=(x,\alpha)$, $q'=(x+a,\alpha)$, a fixed, and $\eta>\nu$ ($\mathscr{L}^1$-clustering). In particular, under this condition the integral in the right-hand side of (2.6) is absolutely convergent.

We need an additional uniformity condition when two particles are sent to infinity. We define

$$M(Q,q_0,q\mid Q',q_0',q')=\rho(Q,q_0,q\mid Q',q_0',q')-\rho(q\mid q')\rho(Q,q_0\mid Q',q_0')$$
$$-\rho(q_0\mid q_0')[\rho(Q,q\mid Q',q')-\rho(q\mid q')\rho(Q\mid Q')]$$
$$-\rho(Q\mid Q')[\rho(q_0,q\mid q_0',q')-\rho(q\mid q')\rho(q_0\mid q_0')] \qquad (2.8)$$

with

$q=(x,\alpha)$, $q'=(x+a,\alpha)$, a fixed

$q_0=(x_0,\alpha_o)$, $q_0'=(x_0+b,\alpha_0)$, b fixed .

By (2.7) this quantity tends to zero as $|x|^{-\eta}$ ($|x_0|^{-\eta}$) when x (x_0) tends to infinity. We then require that

$$M(Q,q_0,q\mid Q',q_0',q)=O\left[\frac{1}{r^\eta}\right],\quad r=\max(|x|,|x_0|)\,. \qquad (2.9)$$

Following the classical analysis, we want to investigate the asymptotic behavior of the Bogoliubov hierarchy as one particle is sent to infinity, i.e., we investigate the equation for

$$\rho(Q,q_0\mid Q',q_0')-\rho(Q\mid Q')\rho(q_0\mid q_0')$$

with

$q_0=(x_0,\alpha_0)$, $q_0'=(x_0+a,\alpha_0)$, $|x_0|\to\infty$.

Using Eqs. (2.6) and (2.8) we find for arbitrary Q,q_0, Q',q_0':

$$-[H(Q,q_0)-H(Q',q_0')][\rho(Q,q_0\mid Q',q_0')-\rho(Q\mid Q')\rho(q_0\mid q_0')]$$
$$=\left[\sum_{i=1}^{k}\phi(q_i,q_0)-\sum_{j=1}^{l}\phi(q_j',q_0')\right]\rho(Q\mid Q')\rho(q_0\mid q_0')$$
$$+\int dq[\phi(q_0,q)-\phi(q_0',q)]\{\rho(q_0\mid q_0')[\rho(Q,q\mid Q',q)-\rho(Q\mid Q')\rho(q\mid q)]+M(Q,q_0,q\mid Q',q_0',q)\}$$
$$+\int dq\left[\sum_{i=1}^{k}\phi(q_i,q)-\sum_{j=1}^{l}\phi(q_j',q)\right]\{\rho(Q\mid Q')[\rho(q_0,q\mid q_0',q)-\rho(q_0\mid q_0')\rho(q\mid q)]+M(Q,q_0,q\mid Q',q_0',q)\}\,. \qquad (2.10)$$

We define now

$$\hat\rho(Q,q\mid Q',q)=\rho(Q,q\mid Q',q)-\rho(Q\mid Q')\rho(q\mid q)+\frac{1}{2}\left[\sum_{i=1}^{k}\delta_{q_iq}+\sum_{j=1}^{l}\delta_{q_j'q}\right]\rho(Q\mid Q') \qquad (2.11)$$

When $Q=Q'$, $\hat\rho(Q,q\mid Q,q)$ is the quantum analog of the excess particle density introduced in the classical case.[2]

Equation (2.10) can be written as

$$-[H(Q,q_0)-H(Q',q_0')][\rho(Q,q_0\mid Q',q_0')-\rho(Q\mid Q')\rho(q_0\mid q_0')]$$
$$=\rho(q_0\mid q_0')\int dq\, e_\alpha e_{\alpha_0}[\phi(x_0-x)-\phi(x_0'-x)]\hat\rho(Q,q\mid Q',q) \qquad (2.12a)$$
$$+\rho(Q\mid Q')\int dq\, e_\alpha\left[\sum_{i=1}^{k}e_{\alpha_i}\phi(x_i-x)-\sum_{j=1}^{l}e_{\alpha_j'}\phi(x_j'-x)\right]\hat\rho(q_0,q\mid q_0',q) \qquad (2.12b)$$
$$+N(Q,q_0\mid Q',q_0') \qquad (2.12c)$$

with

$$N(Q,q_0\mid Q',q_0')=\int dq\, e_\alpha e_{\alpha_0}[\phi(x_0-x)-\phi(x_0'-x)]M(Q,q_0,q\mid Q',q_0',q) \qquad (2.13a)$$
$$+\int dq\, e_\alpha\left[\sum_{i=1}^{k}e_{\alpha_i}\phi(x_i-x)-\sum_{j=1}^{l}e_{\alpha_j'}\phi(x_j'-x)\right]M(Q,q_0,q\mid Q',q_0',q)\,. \qquad (2.13b)$$

This equation (2.12) will be the starting point of the derivation of the sum rules.

III. SUM RULES FOR CHARGED SYSTEMS

In this section, we treat a system of charged particles with pure Coulomb interactions (2.1), or with Coulomb interactions plus a strictly finite range potential. The latter is certainly needed for stability if all species have the Bose statistics. The one-component jellium (with either Bose or Fermi statistics) is also included in our discussion. Except for the uniform neutralizing background of jellium systems, there are no external forces acting on the particles. The state is assumed to be *gauge invariant* and *invariant under translations,* i.e., (2.3) and (2.5) hold for the RDM. In this case the average potential ϕ_ρ in Eq. (2.6) is independent of x and can be included in the chemical potential.

The l-sum rules are exact relations between the RDM which are expressed as follows in three dimensions:

$$\int dx \sum_\alpha e_\alpha |x|^l Y_{lm}(\hat{x})\hat{\rho}(Q,q\,|\,Q',q)=0 \;, \tag{3.1}$$

where $Y_{lm}(\hat{x})$, $\hat{x}=x/|x|$ are the spherical harmonics. For $Q=Q'$ (3.1) has thus exactly the same form as the classical l-sum rules.[3]

We first establish the $l=0$ sum rule for arbitrary ν under the clustering conditions (2.7) and (2.9). It can be written equivalently as

$$C(Q)\rho(Q\,|\,Q')+\int dq\, e_\alpha[\rho(Q,q\,|\,Q',q) -\rho(Q\,|\,Q')\rho(q\,|\,q)]=0 \;. \tag{3.2}$$

We shall then proceed by induction for arbitrary l.

Let $F(x_0,x_0',Q,Q')$ be a function which is twice differentiable and has compact support in all its arguments x_0, x_0', x_i, x_j', and let $\hat{u}$ be a fixed unit vector. We multiply Eq. (2.12) by $\lambda^{\nu-1}F(x_o-\lambda\hat{u},x_o'-\lambda\hat{u},Q,Q')$, integrate over all variables, and then take the limit $\lambda\to\infty$. After integration by parts, and using the invariance under translations, the left-hand side of Eq. (2.12) is

$$-\int dx_0dx_0'dQ\,dQ'\{[H(Q,q_0)-H(Q',q_0')]F(x_0,x_0',Q,Q')\} \times\lambda^{\nu-1}[\rho(Q;x_0+\lambda\hat{u},\alpha_0\,|\,Q';x_0'+\lambda\hat{u},\alpha_0)-\rho(x_0,\alpha_0\,|\,x_0',\alpha_0)\rho(Q\,|\,Q')] \;. \tag{3.3}$$

When (2.7) holds with $\eta>\nu$, this term tends to zero as $\lambda\to\infty$ by dominated convergence.

By using translation invariance again, the term (2.12a) gives

$$\int dx_0dx_0'dQ\,dQ'F(x_0,x_0',Q,Q')e_{\alpha_0}\rho(x_0,\alpha_0\,|\,x_0',\alpha_0)\left\{\lambda^{\nu-1}\int dq\,e_\alpha[\phi(x_0+\lambda\hat{u}-x)-\phi(x_0'+\lambda\hat{u}-x)]\hat{\rho}(Q,q\,|\,Q',q)\right\} \;. \tag{3.4}$$

Since

$$\lim_{\lambda\to\infty}\lambda^{\nu-1}[\phi(x_1+\lambda\hat{u})-\phi(x_2+\lambda\hat{u})]=-(x_1-x_2)\cdot\hat{u}$$

lemma 1 shows that the large curly brackets in (3.4) tends to

$$-e_{\alpha_0}\rho(x_0,\alpha_0\,|\,x_0',\alpha_0)(x_0-x_0')\cdot\hat{u}\int dq\,e_\alpha\hat{\rho}(Q,q\,|\,Q',q) \tag{3.5}$$

and, in (3.4), the limit can be taken under the integral by dominated convergence.

By using gauge and translation invariance the term (2.12b) becomes

$$\int dx_0dx_0'dQ\,dQ'F(x_0,x_0',Q,Q')\rho(Q\,|\,Q') \times\left\{\lambda^{\nu-1}\int dq\,e_\alpha\left[\sum_{i=1}^{k}e_{\alpha_i}[\phi(\lambda\hat{u}+x-x_i)-\phi(\lambda\hat{u}+x)]\right.\right., \left.\left.-\sum_{j=1}^{l}e_{\alpha_j'}[\phi(\lambda\hat{u}+x-x_j')-\phi(\lambda\hat{u}+x)]\right]\hat{\rho}(x_0,\alpha_0,q\,|\,x_0',\alpha_0,q)\right\} \;. \tag{3.6}$$

By the lemma 1, the large curly brackets converges to

$$\left[\sum_{i=1}^{k}e_{\alpha_i}x_i-\sum_{j=1}^{l}e_{\alpha_j'}x_j'\right]\cdot\hat{u}\int dq\,e_\alpha\hat{\rho}(x_0,\alpha_0,q\,|\,x_0',\alpha_0,q) \tag{3.7}$$

as $\lambda\to\infty$ and the term (3.6) converges accordingly.

Finally, with the same arguments, the condition (2.9) and the lemma 2, one gets for the term (2.12c):

$$\lim_{\lambda\to\infty}\lambda^{\nu-1}\int dx_0\int dx_0'F(x_0,x_0',Q,Q')N(Q;x_0+\lambda\hat{u},\alpha_0\,|\,Q';x_0'+\lambda\hat{u},\alpha_0)=0 \;. \tag{3.8}$$

Since $F(x_0,x_0',Q,Q')$ is arbitrary, we must conclude from (3.3)–(3.8) that for all $\hat{u}$:

$$-\hat{u}\cdot(x_0-x_0')e_{\alpha_0}\rho(q_0\mid q_0')\int dq\, e_\alpha\hat{\rho}(Q,q\mid Q',q)+\hat{u}\cdot\left[\sum_{i=1}^{k}e_{\alpha_i}x_i-\sum_{j=1}^{l}e_{\alpha_j'}x_j'\right]\rho(Q\mid Q')\int dq\, e_\alpha\hat{\rho}(q_0,q\mid q_0',q)=0\ . \tag{3.9}$$

Taking in particular $\hat{u}\cdot(x_0-x_0')=0$, $\int dq\, e_\alpha\hat{\rho}(x_0,\alpha_0,q\mid x_0',\alpha_0,q)=0$ for all x_0,x_0', and therefore

$$\int dq\, e_\alpha\hat{\rho}(Q,q\mid Q',q)=0 \quad \text{for all } Q,Q'\ .$$

We establish now the l-sum rules for $l\neq 0$ and $\nu=3$. Assume that the conditions (2.7) and (2.9) hold with $\eta>\nu+l$ and that the sum rules (3.1) are satisfied for $k=0,1,\ldots,l-1$. To establish the l-sum rule, we multiply Eq. (2.12) by $\lambda^{\nu+l-1}$ and average it with the function $F(x_0-\lambda\hat{u},x_0'-\lambda\hat{u},Q,Q')$ as before.

The multipole expansion of the Coulomb potential gives the identity for $|x|<|x_0|$

$$\frac{(-1)^k}{k!}\partial_{i_1\cdots i_k}\left[\frac{1}{|x_0|}\right]x^{i_1}\cdots x^{i_k}=\frac{4\pi}{2k+1}\sum_{m=-k}^{k}\frac{|x|^k}{|x_0|^{k+1}}Y_{km}^*(\hat{x}_0)Y_{km}(\hat{x}) \tag{3.10}$$

and thus by the recursion hypothesis

$$\partial_{i_1\cdots i_k}\left[\frac{1}{|x_0|}\right]\int dq\, e_\alpha x^{i_1}\cdots x^{i_k}\hat{\rho}(Q,q\mid Q',q)=0,\quad k=0,\ldots,l-1\ . \tag{3.11}$$

Let

$$R_{l-1}(x_0,x_0',x)=\frac{1}{|x_0-x|}-\frac{1}{|x_0'-x|}-\sum_{k=0}^{l-1}\frac{(-1)^k}{k!}x^{i_1}\cdots x^{i_k}\partial_{i_1\cdots i_k}\left[\frac{1}{|x_0|}-\frac{1}{|x_0'|}\right]$$

be the rest of the Taylor expansion of $1/|x_0-x|-1/|x_0'-x|$ around $x=0$.

Using (3.11) we subtract in the large curly brackets of (3.4) and (3.6) the $(l-1)$ first terms of the Taylor expansion of the Coulomb potential; since in the limit $\lambda\to\infty$ the finite-range contribution is zero we can ignore it and replace the large curly brackets of (3.4) and (3.6) by

$$\lambda^{\nu+l-1}\int dq\, e_\alpha R_{l-1}(x_0+\lambda\hat{u},x_0'+\lambda\hat{u},x)\hat{\rho}(Q,q\mid Q',q) \tag{3.12}$$

and

$$\lambda^{\nu+l-1}\int dq\, e_\alpha\left[\sum_{i=1}^{k}e_{\alpha_i}R_{l-1}(\lambda\hat{u}-x_i,\lambda\hat{u},-x)-\sum_{j=1}^{l}e_{\alpha_j'}R_{l-1}(\lambda\hat{u}-x_j',\lambda\hat{u},-x)\right]\cdot\hat{\rho}(x_0,\alpha_0,q\mid x_0',\alpha_0,q)\ . \tag{3.13}$$

By using the clustering conditions and lemma 2, the terms (3.3) and (3.8) (with $\lambda^{\nu-1}$ replaced by $\lambda^{\nu+l-1}$) vanish in the limit $\lambda\to\infty$.

Then using lemma 1 and the fact that

$$\lim_{\lambda\to\infty}\lambda^{\nu+l-1}\partial_{i_1\cdots i_l}\left[\frac{1}{|x_0+\lambda\hat{u}|}-\frac{1}{|x_0'+\lambda\hat{u}|}\right]=d_{i_1\cdots i_l j}(\hat{u})(x_0-x_0')^j \tag{3.14}$$

with $d_{i_1\cdots i_l}(\hat{u})=\partial_{i_1\cdots i_l}(1/|x|)_{x=\hat{u}}$, i.e.,

$$\lim_{\lambda\to\infty}\lambda^{\nu+l-1}R_{l-1}(x_0+\lambda\hat{u},x_0'+\lambda\hat{u},x)=\frac{(-1)^l}{l!}d_{i_1\cdots i_l j}(\hat{u})x^{i_1}\cdots x^{i_l}(x_0-x_0')^j$$

we conclude from (3.12)—(3.14) that

$$(-1)^l e_{\alpha_0}\rho(x_0,\alpha_0\mid x_0',\alpha_0)d_{i_1\cdots i_l j}(\hat{u})(x_0-x_0')^j\int dq\, e_\alpha x^{i_1}\cdots x^{i_l}\hat{\rho}(Q,q\mid Q',q)$$
$$-\rho(Q\mid Q')\left[\sum_{i=1}^{k}e_{\alpha_i}x_i-\sum_{j'=1}^{l}e_{\alpha_{j'}'}x_{j'}'\right]^j d_{i_1\cdots i_l j}(\hat{u})\int dq\, e_\alpha x^{i_1}\cdots x^{i_l}\rho(x_0,\alpha_0,q\mid x_0',\alpha_0,q)=0\ . \tag{3.15}$$

We shall show below that each of the two terms (3.15) vanishes; therefore, choosing the third axis parallel to x_0-x_0':

$$d_{i_1 \cdots i_l 3}(\hat{u})(x_0^3 - x_0'^3) \int dq\, e_\alpha x^{i_1} \cdots x^{i_l} \hat{\rho}(Q,q \mid Q',q) = 0 \tag{3.16}$$
$$= (x_0^3 - x_0'^3) \sum_{m=-l}^{l} C_{lm} Y_{l+1,m}(\hat{u}) \int dq\, e_\alpha |x|^l Y_{lm}(\hat{x}) \hat{\rho}(Q,q \mid Q',q) ,$$

where C_{lm} are nonzero constants. The last equality (3.16) is established in Appendix B. Since $\hat{u}$ is arbitrary and the spherical harmonics are linearly independent, the l-sum rules follow.

Equation (3.16) obviously holds for the diagonal part of the RDM since the second term of (3.15) vanishes when $Q=Q'$. To prove (3.16) when $Q \neq Q'$, we first remark that for l odd and the particular choice $Q=(x_0,\alpha_0)$ and $Q'=(x_0',\alpha_0)$ in (3.15), both terms are identical. It follows that (3.16) holds for l odd and general Q and Q'. For l even, (3.16) is also true if the state is invariant under time reflection or space inversion. The first term of (3.15) is then invariant under the exchange of Q and Q' [time reflection, see (2.4)] or under the transformation $x_i \to -x_i, x_j' \to -x_j'$ (space inversion) whereas the second term of (3.15) changes its sign in both cases. This implies again (3.16).

We summarize our results for stationary, gauge and translation invariant states of charged quantum systems in $\mathbb{R}^\nu$, $\nu \geq 2$, in the following proposition.

Proposition:

If the clustering properties (2.7),(2.9) hold with $\eta > \nu + l$ then

(i) the diagonal part of the RDM satisfy the sum rules (3.2) for $k=0,\ldots,l$;

(ii) when the state is invariant under time reflection or space inversion, the off-diagonal RDM satisfy also the sum rules (3.2) for $k=0,\ldots,l$.

Comments.

(1) We have carried out the proof for $l \neq 0$ in three dimensions, but the two-dimensional case is treated in the same way. In one dimension, however, only the $l=0$ sum rule can be established. This is due to the fact that for the one-dimensional Coulomb potential $-|x|$ all the terms of the expansion of $-|x_0 - x| + |x_0' - x|$ for large $|x_0|, |x_0'|$ vanish except the first one, i.e., the limit (3.14) is zero for $l \geq 1$. Hence nothing can be concluded in this case for $l \geq 1$. We gave the proof for the Coulomb case plus a finite range potential. It is clear that the asymptotic form (3.14) remains the same for all l if an exponentially decaying potential is added, and the same proposition holds true. This would however not be the case with an additional potential decaying as some inverse power.

(2) Notice that the terms (2.12b), (2.13b) vanish when $Q=Q'$; gauge and translation invariance has been used only in these terms for $Q \neq Q'$. Therefore, gauge invariance is not needed in the proof for the diagonal part of the RDM. The diagonal part of the RDM satisfies also the sum rules in inhomogeneous Coulomb systems submitted to localized fields or bounded by hard walls (as the semi-infinite system) provided that the state has suitably fast clustering properties. In fact, when $Q=Q'$, one can prove the sum rules for general domains $\mathscr{D} \subset \mathbb{R}^\nu$ and external fields as in the classical case under exactly the same assumptions as in Ref. 2.

(3) The implications of the sum rules on the charge, potential, and field fluctuations are the same as in the classical case.[6,7] In particular, if

$$S(x) = \sum_{\alpha,\beta} e_\alpha e_\beta [\rho(x,\alpha;0,\beta \mid x,\alpha;0,\beta) - \rho(0,\alpha \mid 0,\alpha)\rho(0,\beta \mid 0,\beta)] + \delta_{\alpha\rho}\delta(x)\rho(0,\alpha \mid 0,\alpha) \tag{3.17}$$

is the (truncated) charge-charge correlation and

$$C_\Lambda = \int_\Lambda dx \sum_\alpha e_\alpha a^*(x,\alpha) a(x,\alpha)$$

is (formally) the charge in the region Λ, under the same assumptions as in Ref. 6, the bulk charge fluctuations behave as the surface $\partial\Lambda$,

$$\lim_{\Lambda \to R^3} \frac{\langle C_\Lambda^2 \rangle}{|\partial\Lambda|} = -\tfrac{1}{4} \int dx\, |x| S(x)$$

and we have a central limit theorem as in proposition 4 of Ref. 6. The analysis of Ref. 7 can be reproduced for the quantum situation. Under the assumptions of Ref. 7, the potential correlations $\langle V(x)V(y) \rangle$ and field correlations $\langle E^i(x)E^j(y) \rangle$ at two points in space are given by the formulas (3.7) and (4.1) of Ref. 7 with the quantum charge correlation (3.17). The potential and field correlations decrease slowly even in phases where particle correlations have a fast clustering, i.e.,

$$\langle V(x)V(0) \rangle = \frac{1}{|x|} \left[-\frac{2\pi}{3} \int dy\, |y|^2 S(y) \right] + o\left[\frac{1}{|x|} \right],$$

$$\langle E^i(x)E^j(0) \rangle = \left[\frac{\delta^{ij} - 3\hat{x}^i \hat{x}^j}{|x|^3} \right] \times \left[-\frac{2\pi}{3} \int dy\, |y|^2 S(y) \right] + o\left[\frac{1}{|x|^3} \right].$$

(4) One can check that the $l=0$ sum rule is equivalent with

$$\lim_{\Lambda \to \mathbb{R}^\nu} (\langle C_\Lambda A \rangle - \langle C_\Lambda \rangle \langle A \rangle) = 0$$

for any local multiparticle observable A (cf. proposition 6 in Ref. 6).

IV. APPLICATION TO NEUTRAL FLUIDS AND CONCLUDING REMARKS

We consider here a translation invariant stationary state of a one-component system of neutral particles with a potential satisfying the condition (2) with $\gamma > \nu$. Following the argument given in Ref. 1 for the corresponding classical case, we show that the correlations cannot decrease faster than $|x|^{-(\gamma+1)}$ if the fluid has a strictly positive compressibility χ_T, i.e., if

$$\chi_T = \rho + \int dx[\rho(x,0\,|\,x,0) - \rho^2] > 0 \tag{4.1}$$

$\rho = \rho(0\,|\,0)$ is the density.

In the absence of external forces, the state obeys the Bogoliubov hierarchy (2.6) [with $\phi_\rho(q) = \rho \int \phi(x)dx$] and the analysis leading to the $l=0$ sum rules (3.2) can be carried through as before. Precisely, consider the particular choice $Q = Q' = \{x_1 = 0\}$ [then the terms (2.12b) and (2.13b) vanish] and assume that (2.7) and (2.9) hold with $\eta > \gamma + 1$. Applying now the lemmas 1 and 2, we find that (3.9) holds, giving in this case ($e_\alpha = 1$)

$$\rho + \int dx[\rho(x,0\,|\,x,0) - \rho^2] = 0 \;. \tag{4.2}$$

This contradicts (4.1). Therefore, the clustering of the RDM (2.7) and (2.9) cannot be faster than $|x|^{-(\gamma+1)}$.

This lower bound is probably not optimal and should be replaced by $|x|^{-\gamma}$. We expect indeed that in the high-temperature (low density) phase, the quantum system behaves in the same way as the classical one where we know that the truncated correlations decay exactly as the potential itself. (See Ref. 12.)

To conclude this section, we give a brief discussion of the situation where the gauge invariance (2.3) may be broken. By allowing $\alpha_0 \neq \alpha_0'$ in (2.10), the terms (2.12a) and (2.13a) are modified, $e_{\alpha_0}[\phi(x_0 - x) - \phi(x_0' - x)]$ being replaced then by $e_{\alpha_0}\phi(x_0 - x) - e_{\alpha_0'}\phi(x_0' - x)$. If we have $\eta > \gamma > \nu$ or $\eta > \nu > \gamma$ in (2.7),(2.9) with $\alpha_0 \neq \alpha_0'$, the asymptotic analysis of Eq. (2.12) gives

$$(e_{\alpha_0} - e_{\alpha_0'})\rho(q_0\,|\,q_0') \int dq\, e_\alpha \hat{\rho}(Q,q\,|\,Q',q) + \rho(Q\,|\,Q')[C(Q) - C(Q')] \int dq\, e_\alpha \hat{\rho}(q_0,q\,|\,q_0',q) = 0 \;. \tag{4.3}$$

In the case of a one-component neutral fluid $\gamma > \nu$ and for the choice $q_0 = q_0' = (0,\alpha_0)$, (4.3) reduces to

$$\rho(Q\,|\,Q')(|Q| - |Q'|)\chi_T = 0 \;. \tag{4.4}$$

Thus $\chi_T > 0$ implies $\rho(Q\,|\,Q') = 0$ when $|Q| \neq |Q'|$. We must therefore conclude that in a state with broken gauge invariance the clustering of the RDM is not faster than the decay of the potential. In fact one knows that the spontaneous breaking of a continuous symmetry is accompanied by a weak clustering for instance as slow as $|x|^{-1}$ in the condensed phase of the Bose gas.[13]

In Coulomb non-gauge-invariant systems ($\gamma = \nu - 2$), we consider first the case where $(e_{\alpha_0} - e_{\alpha_0'})\rho(q_0\,|\,q_0') \neq 0$ for some species α_0, α_0'. Equation (4.3) with $Q = \{q_0\}$, $Q' = \{q_0'\}$ implies

$$\int dq\, e_\alpha \rho(q_0,q\,|\,q_0',q) = 0$$

and hence also

$$\int dq\, e_\alpha \hat{\rho}(Q,q\,|\,Q',q) = 0$$

for all Q,Q': we find again the $l=0$ sum rules. If $(e_{\alpha_0} - e_{\alpha_0'})\rho(q_0\,|\,q_0') = 0$ for all α_0, α_0' (but $\rho(Q\,|\,Q')[C(Q) - C(Q')] \neq 0$ for some Q,Q') Eq. (4.3) reduces to

$$\rho(Q\,|\,q')[C(Q) - C(Q')] \int dq\, e_\alpha \hat{\rho}(q_0,q\,|\,q_0',q) = 0 \tag{4.5}$$

and thus we have the $l=0$ sum rule

$$\int dq\, e_\alpha \hat{\rho}(q_0,q\,|\,q_0',q) = 0 \;.$$

However, to obtain the $l=0$ sum rule for general Q and Q' we need the stronger clustering condition $\eta > \nu + 1$. Indeed Eq. (4.5) can be used to write (2.11b) in the form (3.6). If $\eta > \nu + 1$, the asymptotic form of (2.11) gives (3.9) with the additional contribution

$$[C(Q) - C(Q')]\rho(Q\,|\,Q')\hat{u} \cdot \int dq\, e_\alpha \hat{\rho}(q_0,q\,|\,q_0',q) \;.$$

Since $\hat{u}$ is arbitrary this implies again the general $l=0$ sum rules.

Proceeding recursively one can show that the l-sum rules for general Q,Q' hold if the clustering is faster than $|x|^{-(\nu+l+1)}$. These considerations are admittedly speculative since states of Coulomb system with broken gauge invariance (if they exist) are not expected to cluster sufficiently fast to allow the assumptions made in the above analysis.

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APPENDIX A

The following lemma concerns the asymptotic expansion of a convolution (see Ref. 2).

Lemma 1. Let $F(x)$ be a locally integrable function on $\mathbb{R}^\nu$, continuously differentiably in a neighborhood of $x = \infty$ with

$$F(x) = O\left[\frac{1}{|x|^\gamma}\right],$$

$$(\partial_i F)(x) = O\left[\frac{1}{|x|^{\gamma+1}}\right] \quad \gamma > 0$$

and $g(x)$ a bounded function such that $g(x) = O(1/|x|^\eta)$. Then for $\eta > \max(\gamma,\nu)$ we have

$$\int F(x-y)g(y)dy = F(x)\int g(y)dy + o\left[\frac{1}{|x|^\gamma}\right].$$

Moreover, if $F(x)$ is continuously differentiable to order $l+1$ in a neighborhood of $x = \infty$ with

$$(\partial^{(k)}_{i_1 \cdots i_k} F)(x) = O\left[\frac{1}{|x|^{\gamma+k}}\right], \quad k = 0,1,\ldots,l+1$$

we have for $0 < \gamma \leq \nu$ and $\eta > \nu + l$, l integer:

$$\int F(x-y)g(y)dy=\sum_{k=0}^{l}\frac{(-1)^k}{k!}(\partial^{(k)}_{i_1\cdots i_k}F)(x)\int dy\, y^{i_1}\cdots y^{i_k}g(y)+o\left[\frac{1}{|x|^{\gamma+l}}\right].$$

Lemma 2. Let $F(x)$ be a locally integrable function on $\mathbb{R}^\nu$ with $F(x)=O(1/|x|^\gamma)$ and $g(x,y)$ a bounded function on $\mathbb{R}^\nu\times\mathbb{R}^\nu$ such that $g(x,y)=O(1/r^\eta)$, $r=\max(|x|,|y|)$. Then for $\eta>\gamma>\nu$, one has

$$\lim_{|x|\to\infty}\left[|x|^\gamma\int dy\,F(x-y)g(x,y)\right]=\lim_{|x|\to\infty}\left[|x|^\gamma\int dy\,F(y)g(x,y)\right]=0$$

and for $0<\gamma\le\nu$ and $\eta>\nu+l$, l integer

$$\lim_{|x|\to\infty}\left[|x|^{\gamma+l}\int dy\,F(x-y)g(x,y)\right]=\lim_{|x|\to\infty}\left[|x|^{\gamma+l}\int dy\,F(y)g(x,y)\right]=0\,.$$

APPENDIX B

Setting

$$\sum_\alpha e_\alpha\hat{\rho}(Q,q\,|\,Q',q)=C(x),\quad a=x_0^3-x_0'^3\,,$$

one has

$$d_{i_1\cdots i_l3}(\hat{u})a\int dx\,x^{i_1}\cdots x^{i_l}C(x)=\frac{a}{l+1}d_{i_1\cdots i_{l+1}}(\hat{u})\int dx\left[\frac{\partial}{\partial x^3}(x^{i_1}\cdots x^{i_{l+1}})\right]C(x)$$
$$=\frac{4\pi a}{(l+1)(2l+1)}\sum_{m=-(l+1)}^{l+1}Y^*_{l+1,m}(\hat{u})\int dx\left[\frac{\partial}{\partial x^3}(|x|^{l+1}Y_{l+1,m}(\hat{x}))\right]C(x)\,, \qquad \text{(B1)}$$

where the last equality follows from (3.10).

The l-order harmonic polynomial is given by

$$|x|^lY_{lm}(\hat{x})=b_{lm}(L_-)^{l-m}(x^1+ix^2)^l\,, \qquad \text{(B2)}$$

where

$$L_-=L^1-iL^2=(x^1-ix^2)\frac{\partial}{\partial x^3}-x^3\left[\frac{\partial}{\partial x^1}-i\frac{\partial}{\partial x^2}\right] \qquad \text{(B3)}$$

and b_{lm} is a normalization constant. (B2) implies $[\partial/\partial x^3,L_-^l]=-2L_-^{l-1}(\partial/\partial x^1-i\partial/\partial x^2)$ and hence

$$\frac{\partial}{\partial x^3}[|x|^lY_{lm}(\hat{x})]=-2b_{lm}L_-^{l-m-1}\left[\frac{\partial}{\partial x^1}-i\frac{\partial}{\partial x^2}\right](x^1+ix^2)^l$$
$$=-2l\frac{b_{lm}}{b_{l-1,m}}|x|^{l-1}Y_{l-1,m}(\hat{x})\,. \qquad \text{(B4)}$$

Inserting (B4) in (B1) leads to (3.16).

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