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Screening of classical charges in quantum Coulomb systems

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We show that the imaginary-time Green's functions of a system of quantum charged particles at equilibrium satisfy a set of sum rules which express the screening of a classical external charge. We also provide a new derivation of the perfect screening property $\lim_{k\to 0}\epsilon^{-1}(k)=0$ where $\epsilon(k)$ is the static dielectric function. The proof relies on exact equations for the Green's functions and certain assumptions of spatial clustering. It is nonperturbative, independent of the statistics, and applies to jellium as well as to multicomponent systems.

I. INTRODUCTION

A fundamental characteristic of homogeneous metallic (or plasma) phases in thermal equilibrium is the divergence of the static dielectric function $\epsilon(k)$ in the long wavelength limit

$$\lim_{k\to 0}\epsilon^{-1}(k)=0 \ . \tag{1.1}$$

This expresses the perfect screening of a static test charge in the system. In the homogeneous one-component quantum plasma (OCP), Eq. (1.1) can be deduced from the exact compressiblity sum rule $\epsilon(k)\cong 1+4\pi e^2|k|^{-2}\rho^2\gamma$ as $|k|\to 0$, γ being the compressibility.[1,2] In general multicomponent systems of quantum charged particles, Eq. (1.1) holds in the Thomas-Fermi or in the random-phase approximation which give the behavior $\epsilon(k)\cong 1+(|k|\lambda)^{-2}$ as $|k|\to 0$, as $|k|\to 0$, λ being the screening length.

The perfect screening relation (1.1) is equivalent to three sum rules for the first moments of the charge-charge Green's function $S_\tau(x)=\langle Q_\tau(x)Q(0)\rangle$:

$$\int dx \int_0^\beta d\tau S_\tau(x)=0 \ , \tag{1.2}$$

$$\int dx\, x \int_0^\beta d\tau S_\tau(x)=0 \ , \tag{1.3}$$

$$\int dx\, |x|^2 \int_0^\beta d\tau S_\tau(x)=-\frac{3}{2\pi} \ . \tag{1.4}$$

$Q(x)$ is the total charge-density operator, $Q_\tau(x)$ is its imaginary-time translate formally defined by $\exp(\tau H)Q(x)\exp(-\tau H)$ and $\langle\ \rangle$ is the thermal average with respect to the system Hamiltonian H in the thermodynamic limit. Because of the neutrality we have $\langle Q(x)\rangle=0$ for all x in a homogeneous state.

The connection between (1.1) and the sum rules (1.2)—(1.4) is the following. The static susceptibility χ, defined as the linear response function of the charge density to an external classical charge distribution,[3] is related to the Fourier transform $\tilde{S}_\tau$ of S_τ by

$$\chi(k)=-\frac{4\pi}{|k|^2}\int_0^\beta d\tau \tilde{S}_\tau(k) \ . \tag{1.5}$$

Since $\epsilon^{-1}(k)=1+\chi(k)$, the perfect screening relation (1.1) reads

$$\int_0^\beta d\tau \tilde{S}_\tau(k)=\frac{1}{4\pi}|k|^2+o(|k|^2) \ . \tag{1.6}$$

By Fourier transform (1.6) is equivalent to (1.2)—(1.4).

In this paper, we provide a generalization of the sum rules (1.2) and (1.3) to a large class of Green functions, expressing the perfect screening of a static classical test charge in the quantum plasma (Sec. III). Then, we give a simple proof of the perfect screening relation (1.4) based on the only assumptions that the Green functions obey the conditions of thermal equilibrium and have a reasonable spatial decay (Sec. IV). The proof is nonperturbative and covers the case of the OCP as well as multicomponent systems. We thus conclude that an homogeneous phase of charged particles is necessarily metallic, in the sense of Eq. (1.1), when the correlations cluster sufficiently fast in space (essentially, if the first and second moments exist).

The new sum rules derived in Sec. III are

$$\int dx\, \mathscr{Y}_l(x) \int_0^\beta d\tau\langle Q_\tau(x)A\rangle=0 \ , \tag{1.7}$$

where $\mathscr{Y}_l$ is a harmonic polynomial of degree l and A is a general local observable. When A is the charge density and $l=0,1$, we recover (1.2) and (1.3) [note that (1.3) holds trivially by spherical symmetry when $A=Q(0)$, but becomes nontrivial for a nonrotationally invariant A].

Our method is analogous to that which was used to establish similar sum rules for the correlations of a classical charged fluid[4,5] and for the reduced density matrices in the quantum case.[6] We show that the relations (1.7) and (1.4) are constraints imposed by the long range of the Coulomb potential which follow necessarily from the structure of the equilibrium equations for the Green's functions. The derivation relies on certain assumptions on the spatial decay of the Green's functions which have so far not been rigorously proven, even at high temperature. In particular, different behaviors can occur according to the type of correlations which are considered. In a plasma phase, one may expect that the function $\int_0^\beta d\tau\langle Q_\tau(x)A\rangle$ involving the correlation of the charge with any other local observable has a fast (at least integrable) decay. But some care has to be exercised for correlations between observables which are not diagonal in the configuration representation. For instance, the current-current density correlations $\langle J_\tau(x)J(0)\rangle|_{\tau=0}$ of the quantum OCP have a nonintegrable decay even when the corresponding classical phase shows Debye screening.[7] The precise relation between the clustering properties and the validity of the sum rules (1.7) is analyzed in Sec. III: in any case, the violation of (1.7) for a local A will imply a slow decay of some correlations. The arguments which are given in Sec. IV for the proof of the perfect screening relation (1.4) are similar to those presented in the classical context[8] where the result equivalent to (1.4) is known as the second-moment Stillinger-Lovett condition.

To conclude this introduction we give a heuristic derivation of (1.4) and (1.7) in the framework of linear response theory. Let $V=e_0\int dx\,|x|^{-1}Q(x)$ be the potential energy due to an external point charge e_0 located at the origin. To first order in e_0, the equilibrium average $\langle A\rangle_{e_0}$ of an observable A in presence of this external charge is

$$\langle A\rangle_{e_0}=\langle A\rangle-e_0\int dx\int_0^\beta d\tau\,|x|^{-1}\langle Q_\tau(x)A\rangle\ . \tag{1.8}$$

If the charge e_0 is screened, the state $\langle\ \rangle_{e_0}$ will differ from the unperturbed state only in a neighborhood of the origin over distances of the order of the screening length λ. Assuming that $\langle A(y)\rangle_{e_0}-\langle A(y)\rangle\simeq c\exp(-|y|/\lambda)$ decreases exponentially fast as $|y|\to\infty$, with $A(y)$ the space translate of A, we conclude from (1.8) and the translation invariance that

$$\int dx\,|x|^{-1}\int_0^\beta d\tau\langle Q_\tau(x)A(y)\rangle = \int dx\,|x+y|^{-1}\int_0^\beta d\tau\langle Q_\tau(x)A\rangle \tag{1.9}$$

decays faster than any inverse power. As this last expression has the form of an electrostatic potential generated by what might be called an excess charge density induced by e_0, we thus conclude from (1.9) that the excess charge $\int_0^\beta d\tau\langle Q_\tau(x)A\rangle$ carries no multipoles, which is exactly the content of the sum rules (1.7).

Moreover, choosing $A=Q(y)$, the perfect screening of e_0, $\int dy\langle Q(y)\rangle_{e_0}=-e_0$, together with neutrality leads to

$$\int dy\int dx\,|x|^{-1}\int_0^\beta d\tau\langle Q_\tau(x)Q(y)\rangle=1\ . \tag{1.10}$$

By translation invariance and the Poisson equation, (1.10) is equivalent to

$$\begin{aligned}1&=\int dy\int dx\,|x-y|^{-1}\int_0^\beta d\tau S_\tau(x)\\ &=\tfrac{1}{6}\int dy\,|y|^2\Delta\int dx\,|x-y|^{-1}\int_0^\beta d\tau S_\tau(x)\\ &=-(2\pi/3)\int dx\,|x|^2\int_0^\beta d\tau S_\tau(x)\ ,\end{aligned} \tag{1.11}$$

which is the sum rule (1.4).

II. GENERAL SETTING

The system consists of s species of quantum particles in dimension $\nu=2,3$ with mass m_α, charge e_α, spin σ, and statistics ε_α, $\alpha=1,\dots,s$ ($\varepsilon=+1$ for bosons, $\varepsilon=-1$ for fermions). The particles interact by means of the Coulomb potential $V(x)=|x|^{-1}$, $\nu=3$ [$V(x)=-\ln x$, $\nu=2$], and may be submitted to the field due to a classical uniform background of charge density ρ_B (jellium). In multicomponent systems (with $\rho_B=0$), at least the species of negative charge obey the Fermi statistics to insure thermodynamic stability. A short range potential may also be added to the pair interaction: all results will be the same.

The charge-density operator and the Hamiltonian are formally defined by

$$Q(x)=\sum_{\alpha=1}^{s}\sum_\sigma e_\alpha a^*(\alpha,\sigma,x)a(\alpha,\sigma,x)+\rho_B\ , \tag{2.1}$$

$$\begin{aligned}H&=K+U\ ,\\ K&=\sum_{\alpha=1}^{s}\int dr\int dr'(r\,|p^2/2m_\alpha|\,r')\,a^*(\alpha,r)a(\alpha,r')\ ,\end{aligned} \tag{2.2}$$

$$U=\tfrac{1}{2}\int dx_1\int dx_2{:}Q(x_1)V(x_1-x_2)Q(x_2){:}\ , \tag{2.3}$$

with the notation $r=(\sigma,x)$, $\int dr\cdots=\int dx\sum_\sigma\cdots$. The colons mean Wick ordering. The creation and annihilation operators satisfy the usual canonical (anti-)commutation relations

$$\begin{aligned}a(\alpha,\sigma_1,x_1)a^*(\alpha,\sigma_2,x_2)-\varepsilon_\alpha a^*(\alpha,\sigma_2,x_2)a(\alpha,\sigma_1,x_1)&=\delta_{\sigma_1\sigma_2}\delta(x_1-x_2)\ ,\\ a(\alpha,\sigma_1,x_1)a(\alpha,\sigma_2,x_2)-\varepsilon_\alpha a(\alpha,\sigma_2,x_2)a(\alpha,\sigma_1,x_1)&=0\ ,\end{aligned} \tag{2.4}$$

and the operators belonging to different species commute.

The imaginary-time Green's functions (ITGF) are defined (in a finite volume system) by

$$\begin{aligned}\langle A_\tau B\rangle&=\Upsilon^{-1}\mathrm{Tr}(e^{+\beta\boldsymbol{\mu}\cdot\mathbf{N}-(\beta-\tau)H}Ae^{-\tau H}B),\quad 0\le\tau\le\beta\\ \boldsymbol{\mu}\cdot\mathbf{N}&=\sum_{\alpha=1}^{s}\mu_\alpha N_\alpha\ ,\end{aligned} \tag{2.5}$$

where μ_α and N_α are the chemical potentials and particle-number operators, and Υ is the grand partition function. A and B belong to the algebra generated by n-body observables of the form

$$\begin{aligned}A=\frac{1}{n!}\int dr_1\cdots dr_n\int dr_1'\cdots dr_n'(r_1,\dots,r_n\,|\,A_\alpha(1,2,\dots,n)\,|\,r_1',\dots,r_n')\\ \times a^*(\alpha,r_1)\cdots a^*(\alpha,r_n)a(\alpha,r_n')\cdots a(\alpha,r_1')\ \text{ for } n=1,2,\dots,\ \alpha=1,\dots,s\ .\end{aligned} \tag{2.6}$$

$A_\alpha(1,2,\dots,n)$ is a local n-body operator for the particles of species α, i.e., its configurational kernel in (2.6) vanishes when some of the x_j or x_j' are outside of a bounded space region.

In this paper we shall assume that the thermodynamic limit of the ITGF (2.5) exists, and we denote the infinite volume ITGF by the same notation $\langle A_\tau B\rangle$ (the existence of the thermodynamic limit of the ITGF can be proven in some cases, charge symmetric systems with Bose statistics[9]).

The infinitely extended state is stationary,

$$\langle A_\tau \rangle = \langle A \rangle , \tag{2.7}$$

and translation invariant,

$$\langle A(x) \rangle = \langle A \rangle , \tag{2.8}$$

$A(x)$ being the space translate of A.

We also assume local neutrality

$$\langle Q(x) \rangle = \sum_{\alpha=1}^{s} e_\alpha \rho_\alpha + \rho_\beta = 0 , \tag{2.9}$$

where $\rho_\alpha = \langle N_\alpha(x) \rangle$ is the density of particles of species α and $N_\alpha(x) = \sum_\sigma a^*(\alpha,\sigma,x)a(\alpha,\sigma,x)$.

It follows from their definition that the finite-volume ITGF obey the basic equations

$$\langle B_\tau A \rangle = \langle A_{\beta-\tau} B \rangle , \tag{2.10}$$

$$\frac{d}{d\tau}\langle B_\tau A \rangle = \langle [H,B]_\tau A \rangle . \tag{2.11}$$

Combining (2.10) and (2.11) leads immediately to

$$\int_0^\beta d\tau \langle [H,B]_\tau A \rangle = \int_0^\beta d\tau \langle A_\tau [H,B] \rangle = \langle [A,B] \rangle . \tag{2.12}$$

From now on, we assume that the infinite-volume ITGF still verify Eq. (2.12) for local A and B. Equation (2.12) for the infinite system, supplemented with the clustering condition (2.15) below, will be the scattering point of our investigation.

Because of the long range of the Coulomb potential, the commutator $[H,B]$ occurring in (2.12) is not local. Working out the left-hand side of (2.12) for a one-body operator of species α (2.6), we find explicitly, with $H = K + U$,

$$\int_0^\beta d\tau \langle A_\tau [K,B] \rangle = \int dr \int dr' (r \,|\, [K_\alpha(1), B_\alpha(1)] \,|\, r') \times \int_0^\beta d\tau \langle A_\tau a^*(\alpha,r) a(\alpha,r') \rangle \tag{2.13}$$

and

$$\int_0^\beta d\tau \langle A_\tau [U,B] \rangle = e_\alpha \int dr_1 \int dr_1' \int dx_2 \int dx_2' (r_1, x_2 \,|\, [V(1,2), B_\alpha(1)] \,|\, r_1', x_2') \times \int_0^\beta d\tau \langle A_\tau {:}a^*(\alpha,r_1) a(\alpha,r_1') Q(x_2){:} \rangle \tag{2.14a}$$

$$= e_\alpha \int dr_1 \int dr_1' (r_1 \,|\, B_\alpha(1) \,|\, r_1') \int dx_2 [V(x_1 - x_2) - V(x_1' - x_2)] \times \int_0^\beta d\tau \langle A_\tau {:}a^*(\alpha,r_1) a(\alpha,r_1') Q(x_2){:} \rangle . \tag{2.14b}$$

We see that the x_2 integral occurring in (2.14b) is absolutely convergent if the Green's functions satisfy the cluster property with respect to the charge

$$\left| \int_0^\beta d\tau \langle A_\tau a^*(\alpha,\sigma,x) a(\alpha,\sigma',x') Q(y) \rangle \right| \le \frac{M}{|y|^{1+\varepsilon}} , \tag{2.15}$$

$\varepsilon > 0$, for fixed x, x', and A.

The expression (2.13) and (2.14) together with the cluster condition (2.15) and their generalizations to n-body observables B, will be taken as definition for the left-hand side of (2.12).

III. SUM RULES FOR THE GREEN'S FUNCTIONS

In this section, we show that the sum rules (1.7) follow from the equilibrium equation (2.12) under appropriate cluster assumptions. We introduce first the truncated correlation in the usual way

$$\langle AB \cdots C \rangle_T = \langle (A - \langle A \rangle)(B - \langle B \rangle) \cdots (C - \langle C \rangle) \rangle . \tag{3.1}$$

The rate of decay of the ITGF will be characterized as follows. For fixed local A and B, with $B(x)$ the translate of B, we assume for the two-point function a bound of the form

$$\left| \int_0^\beta d\tau \langle A_\tau B(x) \rangle_T \right| \le \frac{c}{|x|^\eta} , \tag{3.2}$$

and for the three-point function

$$\left| \int_0^\beta d\tau \langle A_\tau B(x) Q(y) \rangle_T \right| \le \frac{M(t)}{|x|^\eta} \tag{3.3}$$

with $t = \min(|y|, |y - x|)$. The conditions on η and the decay of $M(t)$ will be specified below. In (3.3), $M(t)$ estimates the joint decay in the three-point truncated function, as the second point y is sent to infinity, A being fixed. Notice that the bounds (3.2) and (3.3) concern only the τ-integrated ITGF and not the ITGF themselves.

We say that a local observable A is diagonal if the n-body operator $A_\alpha(1,2,\ldots,n)$ is diagonal (i.e., acts multiplicatively) in the configuration representation (like the charge and particle densities, the potential, etc.). Typical nondiagonal observables correspond to functions of momenta of the particles. In the sequel we shall specifically use a local approximation of the current associated with a species α. This is formally defined by

$$J_f = \frac{e_\alpha}{m_\alpha} \int dr \int dr' (r \,|\, (pf + fp)/2 \,|\, r') \times a^*(\alpha,r) a(\alpha,r') . \tag{3.4}$$

$p = -i\hbar\nabla$ is the momentum operator and $f(x)$ is a smooth function of the position (spin independent) with compact support.

We treat separately in propositions 1 and 2 the $l=0$ sum rule (charge sum rule) and the higher-order sum rules $l\geq 1$. The charge sum rule holds under weak clustering assumptions formulated in proposition 1, whereas stronger cluster properties are needed to establish the higher-order sum rules.

Proposition 1. Let A be a given local observable. Assume that

(i) for any one-body local B, (3.2) and (3.3) hold with $\eta>\nu-1$ and $\int_0^\infty dt M(t)<\infty$;

(ii) when $B(x)=Q(x)$, (3.2) holds with $\eta>\nu$;

(iii) $\rho_\alpha=\langle N_\alpha(x)\rangle\neq 0$ for some α, $\alpha=1,\dots,s$, then the charge sum rule

$$\int dx \int_0^\beta d\tau \langle Q_\tau(x)A\rangle=\int dx \int_0^\beta d\tau\langle A_\tau Q(x)\rangle=0$$

is true.

Proof of proposition 1. We write Eq. (2.12) for the given A and for $B=J_f(x)$,

$$\int_0^\beta d\tau\{\langle A_\tau[H,J_f(x)]\rangle-\langle A_\tau\rangle\langle[H,J_f(x)]\rangle\} \\ =\langle[A,J_f(x)]\rangle \quad (3.5)$$

and investigate its asymptotic behavior as $x\to\infty$. In (3.5), the truncation of the Green's function in the τ integrand can be introduced freely since $\langle[H,J_f(x)]\rangle=0$ by the stationarity of the state. We work out explicitly the terms of (3.5) with the help of (2.13) and (2.14), noting that

$$[V(x_1-x_2),\tfrac{1}{2}[p_1 f(x_1)+f(x_1)p_1]] \\ =-i\hbar F(x_1-x_2)f(x_1)\ ,$$

where $F(x)=-\nabla V(x)$ is the force.

Using also the translation invariance we find

$$\langle[A,J_f(x)]\rangle=\int_0^\beta d\tau\langle A_\tau[K_\alpha,J_f](x)\rangle_T \quad (3.6a)$$

$$-i\hbar\frac{e_\alpha^2\rho_\alpha}{m_\alpha}\int dx_1\int dx_2 f(x_1)F(x_1+x-x_2) \\ \times\int_0^\beta d\tau\langle A_\tau Q(x_2)\rangle \quad (3.6b)$$

$$-i\hbar\frac{e_\alpha^2}{m_\alpha}\int dx_1\int dx_2 f(x_1)F(x_1+x-x_2) \\ \times\int_0^\beta d\tau\langle A_\tau{:}N_\alpha(x_1+x)Q(x_2){:}\rangle_T\ . \quad (3.6c)$$

We set $x=\lambda\hat{u}$ for a fixed unit vector $\hat{u}$ and let $\lambda\to\infty$ in (3.6). Since the asymptotic form of $F(x_1+\lambda\hat{u}-x_2)$ is $\hat{u}\lambda^{-(\nu-1)}$, it follows from the assumption (ii) (see lemma 1 of Ref. 6) that the term (3.6b) behaves as

$$-i\hbar\frac{e_\alpha^2\rho_\alpha}{m_\alpha}\left[\int dx_1 f(x_1)\right]\frac{\hat{u}}{\lambda^{\nu-1}} \\ \times\int dx_2\int_0^\beta d\tau\langle A_\tau Q(x_2)\rangle+o\left[\frac{1}{\lambda^{\nu-1}}\right]. \quad (3.7)$$

All the other terms in Eq. (3.6) vanish faster than $\lambda^{-(\nu-1)}$: the commutator $[A,J_f(\lambda\hat{u})]$ vanishes for λ large enough since both A and J_f are local. The commutator $[K_\alpha,J_f]$ is the second quantized of the (nondiagonal) one-body operator

$$\frac{e_\alpha}{m_\alpha}\left[\frac{p_\alpha^2}{2m_\alpha},\frac{pf+fp}{2}\right] \\ =-i\hbar\frac{e_\alpha}{4m_\alpha^2}[p(p\cdot\nabla f+\nabla f\cdot p)+(p\cdot\nabla f+\nabla f\cdot p)p]\ .$$

Thus the clustering assumption (i) implies that the term (3.6a) is $o(\lambda^{-(\nu-1)})$ as $\lambda\to\infty$. Finally an application of lemma 1 of Appendix A enables us to conclude with (i) that (3.6c) is also $o(\lambda^{-(\nu-1)})$. Therefore, the coefficient of $\lambda^{-(\nu-1)}$ in (3.7) has to vanish, giving the result of the proposition.

Remark (a). Assumptions (i) and (ii) specify different forms of asymptotic decay according to the type of the observables involved in the Green functions (3.2) and (3.3): the assumption of integrable clustering enters only in (ii) for the charge whereas the correlation between two nondiagonal observables may show a nonintegrable clustering even in the plasma phase, as allowed by (i) (to order $\hbar^2$, equilibrium correlations of the current density decay only as $1/|x|^3$ in the OCP[8]).

Remark (b). It is necessary for this proof to choose a nondiagonal B: therefore, for a general A, an assumption on the clustering of correlations between nondiagonal observables can not be avoided. However, the proof does not depend on the specific choice $B=J_f$.

We now give conditions for the validity of the higher-order sum rules.

Proposition 2. Assume that for a diagonal local A

(i) for one-body local B (3.2) and (3.3) hold with $M(t)=O(1/t^\eta)$ and $\eta>\nu+l$, l being a non-negative integer;

(ii) $\rho_\alpha\neq 0$ for some α, $\alpha=1,\dots,s$. Then the multipolar sum rules

$$\int dx\,\mathcal{Y}_k(x)\int_0^\beta d\tau\langle Q_\tau(x)A\rangle \\ =\int dx\,\mathcal{Y}_k(x)\int_0^\beta d\tau\langle A_\tau Q(x)\rangle=0$$

are true for $k=0,1,\dots,l$. $\mathcal{Y}_k$ is a harmonic polynomial of degree k.

Remark (c). Proposition 2 is formulated for diagonal A so that assumption (i) involves no correlations between pairs of nondiagonal observables. If (i) holds also for a general A, the same result will follow.

The mathematical details of the proof of proposition 2 are similar to those for the reduced density matrices given in Sec. III of Ref. 6. We give only a brief sketch here.

Setting $h(x)=\int_0^\beta d\tau\langle A_\tau Q(x)\rangle$, lemma 1 of Ref. 6 gives the multipole expansion

$$\int dz\,F(\lambda\hat{u}-z)g(z) \\ =\sum_{k=0}^{l}\frac{(-1)^k}{k!}(\partial_{i_1\cdots i_k}F)(\lambda\hat{u}) \\ \times\int dz\,z^{i_1}\cdots z^{i_k}g(z)+o\left[\frac{1}{\lambda^{\nu-1}}\right]. \quad (3.8)$$

Proceeding by induction and assuming that the multipoles of $g(z)$ vanish for $k=0,1,\ldots,l-1$, the term (3.6b) behaves as

$$-i\hbar\frac{e_\alpha^2\rho_\alpha}{m_\alpha}\left[\int dx_1 f(x_1)\right]\frac{(-1)^l}{l!}(\partial_{i_1}\cdots{}_{i_l}F)(\lambda\hat{u})\times\int dz\, z^{i_1}\cdots z^{i_l}h(z)+o\left[\frac{1}{\lambda^{\nu-1}}\right]. \tag{3.9}$$

By (ii) and lemma 2 of Ref. 6, all other terms in Eq. (3.6) are $o(1/\lambda^{\nu-1})$. Introducing for a fixed j, $1\le j\le\nu$,

$$\partial_{i_1}\cdots{}_{i_l}F^j(\lambda\hat{u})=-\frac{1}{\lambda^{\nu-1}}\partial_{i_1}\cdots{}_{i_l j}\left[\frac{1}{|x|}\right]\Bigg|_{x=\hat{u}},$$

we must conclude that

$$\partial_{i_1}\cdots{}_{i_l j}\left[\frac{1}{|x|}\right]\Bigg|_{x=\hat{u}}\int dz\, z^{i_1}\cdots z^{i_l}h(z)=0 .$$

Then the same argument as in Appendix B of Ref. 6 implies that the lth-order multipole of $h(z)$ vanishes.

The two following sum rules will play a particular role in establishing the perfect screening relation in Sec. IV. The first one is the charge sum rule

$$\int dx\int_0^\beta d\tau\langle Q_\tau(x)K^{jj}(0)\rangle=0 , \tag{3.10}$$

for the non-diagonal local observable

$$K^{ij}(y)=\int dx\langle x\,|p^ip^j|\,y\rangle\sum_\sigma a^*(\alpha,\sigma,x)a(\alpha,\sigma,y) \tag{3.11}$$

[$\sum_j^\nu K^{jj}(y)$ can be interpreted as a kinetic energy density]. The second one is the dipole sum rule for the diagonal $A=N_{\alpha_1}(x_1)N_{\alpha_2}(x_2)$ (the product of two-particle densities)

$$\int dx\, x\int_0^\beta d\tau\langle Q_\tau(x)N_{\alpha_1}(x_1)N_{\alpha_2}(x_2)\rangle=0 . \tag{3.12}$$

IV. PERFECT SCREENING

In this section, the perfect screening rule (1.4) is deduced from the Eq. (2.12) for the Green's function with the help of a special choice of the observables $A=D_R$ and $B=J_R$. D_R and J_R are the local polarization and "current" associated with a sphere of radius R. We define J_R as in (3.4) with the smooth cutoff function

$$f(x)=\begin{cases}1, & |x|\le R\\ 0, & |x|>R+1,\end{cases} \tag{4.1}$$

and we set

$$D_R=\int dx\, xg(x)Q(x) \tag{4.2}$$

with a smooth $g(x)$,

$$g(x)=h\left[\frac{x}{R}\right],\qquad h(x)=\begin{cases}1, & 0\le|x|\le 1\\ 0, & |x|\ge 2 .\end{cases} \tag{4.3}$$

Proposition 3. If the assumptions of proposition 1 are satisfied for $A=K^{ij}(0)$, $i,j=1,\ldots,\nu$, (3.11), and those of propositions 2 for $A=N_{\alpha_1}(x_1)N_{\alpha_2}(x_2)$, $l=0,1$, and if the second moment of $\int_0^\beta d\tau\, S_\tau(x)$ is finite, then the perfect screening rule (1.4) is true.

Proof of proposition 3. We write Eq. (2.12) with $A=D_R^j$ and $B=J_R^j$ for a fixed direction j, $1\le j\le\nu$:

$$\frac{1}{\Sigma_\nu R^\nu}\langle[D_R^j,J_R^j]\rangle=\frac{1}{\Sigma_\nu R^\nu}\int_0^\beta d\tau\langle D_{R,\tau}^j[K,J_R^j]\rangle \tag{4.4a}$$

$$+\frac{1}{\Sigma_\nu R^\nu}\int_0^\beta d\tau\langle D_{R,\tau}^j[U,J_R^j]\rangle , \tag{4.4b}$$

Σ_ν is the volume of the sphere of radius 1 in $\mathbb{R}^\nu$. Letting $R\to\infty$, we show that (4.4) reduces to the perfect screening relation (1.4).

Evaluating the commutator in the left-hand side of (4.4) gives

$$\lim_{R\to\infty}\frac{1}{\Sigma_\nu R^\nu}\langle[D_R^j,J_R^j]\rangle$$
$$=\frac{i\hbar e_\alpha^2\rho_\alpha}{m_\alpha}\lim_{R\to\infty}\frac{1}{\Sigma_\nu R^\nu}\int dx\, f(x)\nabla^j(x^jg(x))$$
$$=\frac{i\hbar e_\alpha{}^2\rho_\alpha}{m_\alpha}\lim_{R\to\infty}\frac{1}{\Sigma_\nu}\int dx\, f(Rx)\nabla^j(x^jh(x))=\frac{i\hbar e_\alpha^2\rho_\alpha}{m_\alpha} . \tag{4.5}$$

This follows by dominated convergence from the fact that

$$\lim_{R\to\infty}f(Rx)=\begin{cases}1, & |x|\le 1\\ 0, & |x|>1\end{cases}$$

and

$$\nabla^j(x^jh(x))=h(x)+x^j\nabla^jh(x)=1$$

for $0\le x\le 1$.

We find in Appendix B that the kinetic energy term (4.4a) is

$$\lim_{R\to\infty}\frac{1}{\Sigma_\nu R^\nu}\int_0^\beta d\tau\langle D_{R,\tau}^j[K,J_R^j]\rangle$$
$$=i\hbar e_\alpha m_\alpha^{-2}\int dx\int_0^\beta d\tau\langle Q_\tau(x)K^{jj}(0)\rangle=0 . \tag{4.6}$$

This quantity vanishes as a consequence of the charge sum rule (3.10).

Introducing the fully truncated three-point function, we find that potential energy term (4.4b) is the sum of two contributions as in (3.6b) and (3.6c)

$$\frac{1}{\Sigma_\nu R^\nu}\int_0^\beta d\tau\langle D^j_{R,\tau}[U,J^j_R]\rangle=-\frac{i\hbar e^2_\alpha\rho_\alpha}{m_\alpha}\frac{1}{\Sigma_\nu R^\nu}\int dx_1dx_2dx_3F^j(x_1-x_2)f(x_1)x^j_3g(x_3)\int_0^\beta d\tau\langle Q_\tau(x_3)Q(x_2)\rangle \tag{4.7a}$$

$$-i\hbar\frac{e^2_\alpha}{m_\alpha}\frac{1}{\Sigma_\nu R^\nu}\int dx_1dx_2dx_3F^j(x_1-x_2)f(x_1)x^j_3g(x_3)$$

$$\times\int_0^\beta d\tau\langle Q_\tau(x_3){:}N_\alpha(x_1)Q(x_2){:}\rangle_T\ . \tag{4.7b}$$

The limit of (4.7b) is (see Appendix B)

$$-i\hbar\frac{e^2_\alpha}{m_\alpha}\int dy\,F^j(y)\int dx\,x^j\int_0^\beta d\tau\langle Q_\tau(x){:}N_\alpha(0)Q(y){:}\rangle_T=0\ , \tag{4.8}$$

which is zero by the dipole sum rule (3.12).

After the change of variables $z=x_1$, $x=x_3-x_1$, $y=x_3-x_2$, the term (4.7a) is

$$-i\hbar\frac{e^2_\alpha\rho_\alpha}{m_\alpha}\int dx\left[\lim_{R\to\infty}\frac{1}{\Sigma_\nu R^\nu}\int dz\,f(z)(z+x)^jg(z+x)\right]\nabla^j_x\int dy\,V(x-y)\int_0^\beta d\tau S_\tau(y)\ . \tag{4.9}$$

To find its limit, we note that with the definitions of f and g

$$\frac{1}{\Sigma_\nu R^\nu}\int dz\,f(z)(z+x)^jg(z+x)$$

$$=\frac{1}{\Sigma_\nu}x^j\int dz\,f(Rz)h\left[z+\frac{x}{R}\right]+\frac{R}{\Sigma_\nu}\int dz\,f(Rz)z^jh\left[z+\frac{x}{R}\right]$$

$$=\frac{1}{\Sigma_\nu}x^j\int dz\,f(Rx)h\left[z+\frac{x}{R}\right]+\frac{R}{\Sigma_\nu}\int dz\,f(Rz)z^j+\frac{1}{\Sigma_\nu}x\cdot\int dz\,f(Rz)z^j(\nabla h)\left[z+\vartheta\frac{x}{R}\right],\quad 0\le\vartheta\le 1\ . \tag{4.10}$$

The first term in (4.10) tends to x^j, the second being independent of x does not contribute to (4.9), and the last one tends to zero [since $(\nabla h)(z)=0$, $|z|\le 1$]. Thus, the limit of (4.9) is

$$-i\hbar\frac{e^2_\alpha\rho_\alpha}{m_\alpha}\int dx\,x^j\nabla^j_x\int dy\,V(x-y)\int_0^\beta d\tau S_\tau(y)$$

$$=i\hbar\frac{e^2_\alpha\rho_\alpha}{m_\alpha}\int dx\int dy\,V(x-y)\int_0^\beta d\tau S_\tau(y)$$

$$=-i\hbar\frac{e^2_\alpha\rho_\alpha}{m_\alpha}\frac{c_\nu}{2\nu}\int dx\,|x|^2\int_0^\beta d\tau S_\tau(x)\ ,$$

$$c_2=2\pi,\quad c_3=4\pi\ , \tag{4.11}$$

where the last line is obtained as in (1.11). This, together with (4.5), (4.6), and (4.8) gives the perfect screening relation (1.4).

V. CONCLUDING REMARKS

As shown in the Introduction, the sum rules (1.7) for the imaginary-time Green's functions express the shielding of external *classical static test charges* in the system. It is important to remark that the ITGF sum rules are conceptually different from those for the reduced density matrices (RDM) discussed in Ref. 6. Since the reduced density matrices describe internal correlations in the systems, the RDM sum rules are linked to the shielding of the system's own charges which are truly *quantum mechanical.*

If the system is treated classically, this distinction does not occur: the excess charge density introduced in Ref. 4 in the classical case can equivalently be interpreted as the induced charge density by an external distribution, or as the charge cloud associated with a specification of a number of the system's particles. But in the quantum-mechanical case, these two types of screening may not be equivalent: they depend on the cluster properties of the ITGF or the RDM which might be different. One could even conjecture that the ITGF, more closely related to classical screening, might have better cluster properties than the RDM. The latter embody necessarily some dynamical correlation between a particle and its cloud since quantum mechanically position and velocity distribution cannot be disentangled.

This point can be illustrated when we compare the susceptibility χ and the structure function $S_0(x)=\langle Q(x)Q(0)\rangle$. Classically, since both quantities are simply proportional in Fourier space, $\chi(k)=-4\pi\tilde{S}_0(k)/|k|^2$, the perfect screening condition (1.1) yields immediately a sum rule for $S_0(x)$ (the second-moment Stillinger-Lovett relation). This remarkable fact is not true in quantum systems: the susceptibility $\chi(k)$ given by (1.6) has no direct relation to $\tilde{S}_0(k)$, and a sum rule for it yields no information on S_0. Apparently, except for the OCP, no exact sum rule [other than the electroneutrality $\int dx\,S_0(x)=0$] is known for the quantum-mechanical structure function. In the OCP, because of the special feature that the mass and charge current are proportional, the plasmon mode $\omega_p=(4\pi e^2\rho/m)^{1/2}$ is undamped in the long-wavelength limit. This results in the second-moment sum rule

$$\int dx\,|x|^2 S_0(x) = -(3/4\pi)\hbar\omega_p \coth(\beta\hbar\omega_p/2)$$

which is specific to the OCP and has the same classical limit as (1.4) (Refs. 2 and 7).

APPENDIX A

Lemma. Let $F(x)=x/|x|^\nu$ be the Coulomb force and $g(x,y)$ be a bounded function on $\mathbb{R}^\nu \times R^\nu$ satisfying

$$|g(x,y)| \le \frac{M(t)}{|x|^\eta},\quad t=\min(|y|,|x-y|)\ ,$$

$$\int_0^\infty dt\, M(t) < \infty\ ,$$

then $\int dy\, F(x-y)g(x,y)=O(|x|^{-\eta})$.

Proof. For a fixed x, we decompose $\mathbb{R}^\nu = D \cup \bar{D}$ into two disjoint domains with $D=\{y \mid |y| \le |y-x|\}$ and $\bar{D}$ its complement. Then we have on D

$$\left|\int_D dy\, F(x-y)g(x,y)\right| \le |x|^{-\eta}\int_D dy\, M(|y|)\,|x-y|^{1-\nu}$$
$$\le |x|^{-\eta}\int_D dy\, M(|y|)\,|y|^{1-\nu}$$
$$\le |x|^{-\eta}\int_{\mathbb{R}^\nu} dy\, M(|y|)\,|y|^{1-\nu} = O(|x|^{-\eta})\ .$$

Similarly, on $\bar{D}$,

$$\left|\int_{\bar{D}} dy\, F(x-y)g(x,y)\right| \le |x|^{-\eta}\int_{\bar{D}} dy\, M(|x-y|)\,|x-y|^{1-\nu}$$
$$\le |x|^{-\eta}\int_{\mathbb{R}^\nu} dy\, M(|y|)\,|y|^{1-\nu} = O(|x|^{-\eta})\ .$$

We apply the lemma to (3.6c) with

$$g(x,y)=\int_0^\beta d\tau \langle A_\tau : N_\alpha(x) Q(y) : \rangle_T\ .$$

Thus (3.6c) is majorized by

$$\hbar e_\alpha^2 m_\alpha^{-1} \int dx_1 f(x_1)\, \mathbb{C}\,|x_1+x|^{-\eta} = o(|x|^{1-\nu})$$

since f has compact support and $\eta > \nu - 1$.

APPENDIX B

Proof of (4.6). For $1 \le i \le \nu$, let

$$K_R^{ij} = \int dx\, dy \tfrac{1}{4} \langle x \mid \{p^i,\{p^j,f\}\} \mid y\rangle \times \sum_\sigma a^*(\alpha,\sigma,x)a(\alpha,\sigma,y)\ ,$$

where $\{a,b\}=ab+ba$ and f is given in (4.1). Some algebra shows that

$$[\,|p|^2/2,(p^j f + f p^j)/2] = \sum_{k=1}^{\nu} [P^k, K^{kj}]\ , \tag{B1}$$

which implies [see (3.11)]

$$[K, J_R^j] = e_\alpha m_\alpha^{-2} \sum_{k=1}^{\nu} [P^k, K_R^{kj}]\ , \tag{B2}$$

where P^k is the generator of the translations. By translation invariance of the state,

$$\langle D_{R,\tau}^j [P^k, K_R^{kj}]\rangle + \langle [P^k, D_{R,\tau}^j] K_R^{kj}\rangle = \langle [P^k, D_{R,\tau}^j K_R^{kj}]\rangle = 0\ . \tag{B3}$$

The left-hand side of (4.6) is, by (B2) and (B3),

$$\frac{1}{\Sigma_\nu R^\nu}\int_0^\beta d\tau \langle D_{R,\tau}^j [K, J_R^j]\rangle = (\Sigma_\nu R^\nu)^{-1} i\hbar e_\alpha m_\alpha^{-2} \times \sum_{k=1}^{\nu}\sum_\sigma \int dx_1 \nabla^k(x_1^j g(x_1)) \int_0^\beta d\tau \langle Q_\tau(x_1) K_R^{kj}\rangle\ . \tag{B4}$$

Writing explicitly the anticommutators, we have

$$K^{kj} = p^k p^j f + i\hbar p^k \nabla^j f/2 + i\hbar p^j \nabla^k f/2 - \hbar^2 \nabla^j \nabla^k f/4\ . \tag{B5}$$

The contribution of the first term of (B5) to (B4) is estimated below. The other terms contain at least a first derivative of f. Since the volume of the support of ∇f is of the order of $R^{\nu-1}$ for large R, they are $O(R^{-1})$ and vanish in the limit $R\to\infty$ (see Appendix 3 of Ref. 7, in fact the terms linear in p do not contribute because of time-reversal invariance). The first contribution to (B4) is

$$(\Sigma_\nu R^\nu)^{-1} i\hbar e_\alpha m_\alpha^{-2} \sum_{k=1}^{\nu} \int dx_1 \nabla^k(x_1^j g(x_1)) \int dx_2 f(x_2) \int_0^\beta d\tau \langle Q_\tau(x_1) K^{kj}(x_2)\rangle$$
$$= i\hbar e_\alpha m_\alpha^{-2} \sum_{k=1}^{\nu} \int_0^\beta d\tau \langle Q_\tau(x) K^{kj}(0)\rangle (\Sigma_\nu R^\nu)^{-1} \int dy\, f(y-x) \nabla^k(y^j g(y)) \tag{B6}$$

by translation invariance and a change of variables. With the definition (4.3), we get

$$\lim_{R\to\infty} (\Sigma_\nu R^\nu)^{-1} \int dy\, f(y-x)\nabla^k(y^j g(y)) = \lim_{R\to\infty} \Sigma_\nu^{-1} \int dz\, f(Rz - x)\nabla^k(z^j h(z)) = \Sigma_\nu^{-1} \int_{|z|\le 1} dz\, \nabla^k(z^j h(z)) = \delta_{kj}\ .$$

Thus by dominated convergence, the limit of (B6) leads to (4.6).

Proof of (4.8). After a change of variables, the term (4.7b) is

$$i\hbar e_\alpha^2 m_\alpha^{-1} \int dy\, F(y) \int dx \int_0^\beta d\tau \langle Q_\tau(x) {:} N_\alpha(0) Q(y){:} \rangle_T \left[(\Sigma_\nu R^\nu)^{-1} \int dz\, f(z)(z+x)^j g(z+x) \right] \tag{B7}$$

and we find, as in (4.10), that the term in the large parentheses tends to x^j as $R\to\infty$. By the cluster assumption, the Green's function is jointly integrable in x and y, hence (4.8) follows by dominated convergence.

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