

Coulomb glass in the random phase approximation

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A three-dimensional model of the electrons localized on randomly distributed donor sites of density n and with the acceptor charge uniformly smeared on these sites, $-Ke$ on each, is considered in the random phase approximation (RPA). For the case $K=1/2$ the free energy, the density of the one-site energies (DOSE) ε , and the pair OSE correlators are found. In the high-temperature region ($e^2 n^{1/3}/T < 1$ (T is the temperature)) RPA energies and DOSE are in a good agreement with the corresponding data of Monte Carlo simulations. Thermodynamics of the model in this region is similar to the one of an electrolyte in the regime of Debye screening. In the vicinity of the Fermi level $\mu=0$ the OSE correlations, depending on $\text{sgn}(\varepsilon^1 \cdot \varepsilon^2)$ and with very slow decoupling law, have been found. The main result is that even in the temperature range where the energy of a Coulomb glass is determined by Debye screening effects, the correlations of the long-range nature between the OSE still exist.

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I. INTRODUCTION

Electron-electron interactions affect considerably the low-temperature behavior of doped semiconductors on both sides of the metal-dielectric transition.¹⁻³ On the dielectric side the Coulomb interaction between the localized electrons makes the density of the one-site excitations (DOSE) to tend to zero as a power law in the vicinity of the Fermi level, as argued by Efros and Shklovskii.³ Because of the DOSE concerns the low-temperature conductivity and tunneling characteristics of doped semiconductors, many investigations^{4,5} were undertaken⁶⁻⁹ to elucidate the nature of this so-called Coulomb correlation gap. The rare analytical results in this area¹⁰⁻¹⁴ are due to the hardness of the problem considered. Today, the only well established analytical results^{12,14} are the temperature dependences $\sim T^{D-1}$ for $D \geq 2$ and $\sim [\ln(1/T)]^{-1}$ for $D=1$ found for $g(\mu)$. As it was shown,¹³ the nonlinear equation¹⁰ for $g(\varepsilon)$ at $T=0$ is based on some vague assumptions about decoupling of OSE correlations. Mogylansky and Raikh¹¹ managed to extend the approach¹⁰ to the case of nonzero temperatures. The base of their method comprises of the Metropolis algorithm¹⁵ adapted to analytical applications at the expense of the two indefinite assumptions. The first one is concerned with the decoupling of the pair OSE correlations. The second one admits the law of Markoff type for the approach to equilibrium in terms of ρ as a formal "time": a charge transfer between the sites with the distances from the interval $(\rho, \rho + d\rho)$ does not influence DOSE found "previously" in terms of ρ as a time. Recently, this approach¹¹ has been extended to include the pair correlations of OSE,¹⁶ and the solution has been found for the two-dimensional case in the first order of the perturbation theory on the pair potential $V(\rho)$, decreasing no slower than $1/\rho^2$ as ρ tends to infinity. In the case of high temperatures the parameter $V(\rho)/T$ plays the role of the small one in the theory.¹⁶ Because the approaches developed are of a qualitative and uncontrolled character it is desirable to compare them to some well established analytical results such as the high-temperature expansions of the free energy

and correlations for the Coulomb glass problem. Meanwhile, it is well known¹⁷ that the development of the free energy or correlations in powers of the parameter $V(\rho)/T$ gives divergent terms in the case where $V(\rho)$ is the Coulomb potential. Mayer's approach to solving this problem¹⁸⁻²¹ is based on a very complicated technique of the redevelopment of terms in series with following resummations aiming to remove divergences from the terms of the new series. Later a quite different approach to this problem, using Fourier components of local densities as so-called "collective" variables (CV's), was elaborated.^{22,23} Compared to Mayer's approach, this one is considerably simpler. The central point of this approach consists of switching from the individual variables to CV's via the corresponding Jacobian. In many cases this Jacobian has the form of the integral on a CV measure with an exponential form as the integrand. An exponent of this integrand should be considered as a part of an action for a statistical mechanics of a nonlinearly self-interacting field. Already in the zero approximation of this self-interaction the well-known random phase approximation (RPA) arises and the following expansion of the exponent gives the cluster expansions for the free energy and correlators.²⁴ Since the thermodynamics of Debye electrolytes^{17,24} in the temperature range

$$\frac{e^2 n^{1/3}}{T} < 1 \quad (1)$$

is well described by RPA, one should expect a similar behavior would take place for the Coulomb glass in this region. It was our goal to investigate thermodynamics of a Coulomb glass (the free energy, DOSE, and the pair OSE correlators) in RPA aiming to have the reliable results in the region where RPA is applicable. In the present paper the Coulomb glass model with $N \cdot (1-K)$ electrons localized on N donor sites and with the acceptor charge $-Ke$ ascribed to each donor site is considered. The energy of the model considered depends as on the donor site configuration $\mathbf{R}=[x_i]_1^N$ so on the charge distribution $m=[m_i]_1^N$:

$$\hat{H}[m] = \frac{1}{2} \sum_{i \neq j} \frac{m_i m_j}{r_{i,j}} + C[m]. \quad (2)$$

Here $m_i = L$ for the neutral and $m_i = -K$ for the ionized site. The whole set $m = [m_i]_1^N$ obeys the electroneutrality condition

$$\sum_1^N m_i = 0. \quad (3)$$

From now on the cap above some variable [e.g., the energy (2)] means \mathbf{R} dependence, and $r_{i,j}$ means the distances between the sites. The expression (2) has been written in dimensionless form with the scales $n^{-1/3}$ for lengths and $e^2 n^{1/3}$ for energies and temperatures. The constant $C[m]$, not depending on \mathbf{R} , has been added into Eq. (2) to remove the $\vec{k} = 0$ Fourier component of the bare Coulomb potential. Actually, the constant $C[m]$ depends only on K , provided the electroneutrality condition (3) is fulfilled; its specific value will be given later. In all calculations concerning with the equilibrium averages we use the Ising spin variables σ_i instead of m_i :

$$2m_i = (1 - 2K) + \sigma_i, \quad \text{where } \sigma_i = \pm 1. \quad (4)$$

The case $K = 1/2$ is the simplest one because summing on the independent Ising spins provides the electroneutrality in the thermodynamic limit.²⁵ In the present work we confine ourselves to the case $K = 1/2$. A side benefit is that the Fermi level $\mu(T, K) = 0$ in this case. This becomes evident if we take into account the invariance of the sums in equilibrium averages with respect to the $K \rightarrow L$ changing. As the consequence, we get two symmetry relations: $F_N(T, K) = F_N(T, L)$, for the free energy, and $\mu(T, K) = -\mu(T, L)$, for the Fermi-level, provided we define last as the derivative of F_N on the number of the electrons $N \cdot (1 - K)$ at N being a constant. Our approach is based on the combination of the CV (Refs. 17, 22, and 23) and the replica²⁶ methods. Besides, we used Monte Carlo (MC) simulations¹⁵ to elucidate the region of RPA applicability.

The remaining part of this paper is organized as follows. In Sec. II we give some background to our approach and find the free energy in RPA. We compare our analytical results to MC simulation data and find good quantitative agreement in the region (1). In Sec. III we present DOSE found in RPA, compare it to MC simulation data and once more get the evidence of the good applicability of RPA in region (1). In Sec. IV we present the formulas for the pair OSE correlators in RPA. Being cumbersome, they, however, have a simple behavior in the asymptotic regime $r > r_d$ (r_d is the screening radius). Quite unexpectedly, it turns out that near the Fermi level $\mu = 0$ in an energy strip of the order $T^{-1/2}$ a very slow decoupling of OSE correlations exists, attractive for OSE of the same signs and repulsive for those of opposite sign. In Sec. V we present a qualitative comparison of our formulas to the ones of Blanter and Raikh.¹⁶ In Sec. VI we formulate our conclusion.

II. BACKGROUND: COLLECTIVE VARIABLES

We present in this section the integral representation for the free energy $F_N(\beta)$ (from now on $\beta = 1/T$). Then we use this representation to get the RPA formula for $F_N(\beta)$ and compare to MC simulation data.

A. Energy in the terms of CV

In the replica approach it is the replicated partition function

$$\overline{\hat{Z}_N^s} = \text{Tr}_N^K \exp\left(-\beta \sum_{a=1}^s \overline{\hat{H}_N(m_a)}\right) \quad (5)$$

which one has to calculate to find then F_N by the formula

$$F_N(\beta, K) = \lim_{s \rightarrow 0} \left(\frac{1 - \overline{\hat{Z}_N^s}}{\beta s} \right). \quad (6)$$

In expression (5): s is an integer, Tr_N^K means the sum over the whole set of charge states $[m_j^a]_1^N, a = 1, 2, \dots, s$, obeying the electroneutrality condition (3) for each a . The overlines in expressions (5) and (6) denote the averaging on the Poisson distribution of the specimens \mathbf{R} :

$$\overline{\mathcal{Q}} = \int \frac{d\vec{x}_1}{V} \int \frac{d\vec{x}_2}{V} \dots \int \frac{d\vec{x}_N}{V} \mathcal{Q}(\vec{x}_1, \vec{x}_2, \dots, \vec{x}_N). \quad (7)$$

We choose as CV's the Fourier components $\hat{Q}_{\vec{k}}$ of the development

$$\hat{Q}(\vec{x}) = \sqrt{\frac{KL}{N}} \sum_{\vec{k} \neq 0} \hat{Q}_{\vec{k}} \exp(i\vec{k}\vec{x}) \quad (8)$$

for the local charge density

$$\hat{Q}(\vec{x}) = \sum_{i=1}^N m_i \delta(\vec{x} - \vec{x}_i). \quad (9)$$

The electroneutrality condition (3) implies $\hat{Q}_{\vec{k}} = 0$ at $\vec{k} = 0$. From now on we work with the regularized Coulomb potential

$$\Phi_c(\vec{x}) = \frac{1}{N} \sum_{\vec{k}} \tilde{\Phi}_{\vec{k}} \exp(i\vec{k}\vec{x}), \quad \tilde{\Phi}_{\vec{k}} = \frac{4\pi}{\vec{k}^2 + \alpha^2}. \quad (10)$$

Besides, all sums $\sum_{\vec{k}}$ and products $\prod_{\vec{k}}$ are considered as having the ultraviolet regularization $|\vec{k}| \leq \Lambda$. We will take the limits $\Lambda \rightarrow \infty$ and $\alpha \rightarrow 0$ only in final results. The insert of the expansion (10) into the formula (2) gives us the energy expression through CV's. The constant in Eq. (2) has to be chosen as

$$C[m] = \tilde{\Phi}_0 \cdot \left(\frac{1}{2N} \sum_{i=1}^N m_i^2 \right) \quad (11)$$

to remove from the energy

$$\hat{H}_N[m] = \sum_k' \nu_k (\hat{Q}_k \hat{Q}_{-k} - 1) \quad (12)$$

the term with $\vec{k}=0$. In expression (12) the stroke above the sum symbol means summing over the half space $\{\vec{k}: 0 < k_x^2 + k_y^2 + k_z^2 \leq \Lambda^2, k_z \geq 0\}$. From now on the presence of the stroke above a symbol of a sum or a product means the action on this half space. The function ν_k entering Eq. (12) is defined as

$$\nu_k = \frac{k_d^2}{\vec{k}^2 + \alpha^2}, \quad k_d^2 = 4\pi\beta KKL. \quad (13)$$

It can be simply proven, using the electroneutrality condition (3) and Ising spins (4), that $C[m] = \frac{1}{2}KL\bar{\Phi}_0$, i.e., it does not actually depend on the charge configuration m . Notwithstanding, we prefer to keep the form (11) since OSE calculation breaks electroneutrality.

B. Jacobian

For the s charge distributions $[m_j^a]_1^N$, with $a=1,2,\dots,s$, on the same specimen \mathbf{R} , we define the real variables \hat{C}_k^a and \hat{S}_k^a as the real and imaginary parts of CV's: $\hat{Q}_k^a = \hat{C}_k^a + i\hat{S}_k^a$. These real variables obey the symmetry relations $\hat{C}_k^a = \hat{C}_{-k}^a$, $\hat{S}_k^a = -\hat{S}_{-k}^a$, so that as functions of \vec{k} they are actually defined on the half space described above. In parallel with the depending on the specimen R CV, we consider the "free" variables $Q_k^a = C_k^a + iS_k^a$, with the same symmetry relations as for the CV with the "hats," and switch to these free variables in the expression (5) for the replicated partition function

$$\begin{aligned} \overline{\hat{Z}_N^s} &= \exp\left(s \cdot \sum_k' \nu_k\right) \\ &\times \text{Tr}_N^K \left[\int dQ \exp\left(-\sum_k' \nu_k \bar{Q}_k \cdot \bar{Q}_{-k}\right) \cdot J(\bar{Q}, \vec{m}) \right] \end{aligned} \quad (14)$$

using the Jacobian

$$J(\bar{Q}, \vec{m}) = \prod_{a=1}^s \prod_k' \delta(C_k^a - \hat{C}_k^a) \cdot \delta(S_k^a - \hat{S}_k^a). \quad (15)$$

The measure dQ in the formula (14) is defined as $dQ = \prod_{a=1}^s \prod_k' dC_k^a \cdot dS_k^a$. In the formulas (14) and (15) \bar{Q}_k and \vec{m}_j mean the vectors in the s -dimensional space and expressions like $\bar{Q}_k \cdot \bar{Q}_{-k}$ mean the scalar products in this space. The exceptional simplicity of the Poisson formula (7) allows us to make the exact averaging in Eq. (15) and get for the Jacobian (15) an integral representation in terms of CV measure in the CV-Fourier space. To do this, we put into using the real fields

$$z^a(\vec{x}) = \frac{1}{\sqrt{KLN}} \sum_{k \neq 0} z_k^a \exp(i\vec{k} \cdot \vec{x}), \quad 1 \leq a \leq s, \quad (16)$$

the real variables p_k^a and q_k^a defined on the half space as $z_k^a = p_k^a + iq_k^a$ and the measure in the CV-Fourier space $dz = \prod_k' (d\vec{p}_k / \pi^s) \cdot (d\vec{q}_k / \pi^s)$. Then, using the integral representation for the δ functions and Poisson averaging (7), we get

$$\begin{aligned} J(\bar{Q}, \vec{m}) &= \int dz \exp\left[-2i \sum_k' (\bar{C}_k \bar{p}_k \right. \\ &\quad \left. + \bar{S}_k \bar{q}_k)\right] \cdot \prod_{j=1}^N \overline{\exp[i\vec{m}_j \cdot \vec{z}(x_j)]}. \end{aligned} \quad (17)$$

In the final step we transform the Jacobian inserting the identity²³

$$\overline{\exp[i\vec{m} \cdot \vec{z}(x)]} = \exp\left[\sum_{n=2}^{\infty} \frac{i^n}{n!} \omega_n(\vec{m} \cdot \vec{z})\right] \quad (18)$$

which expresses the left-hand side of Eq. (18) through the *irreducible sums*

$$\begin{aligned} \omega(\vec{z} \cdot \vec{m}) &= \left(\frac{1}{KLN}\right)^{n/2} \sum_{\langle k_1+k_2+\dots+k_n \rangle=0} (\vec{m} \vec{z}_{k_1}) \\ &\quad \times (\vec{m} \vec{z}_{k_2}) \cdots (\vec{m} \vec{z}_{k_n}). \end{aligned} \quad (19)$$

In Eq. (19) the symbol $\langle k_1+k_2+\dots+k_n \rangle=0$ means that $k_{i_1}+k_{i_2}+\dots+k_{i_p} \neq 0$ for *any* subset, but $[k_1, k_2, \dots, k_n]$ itself. By inserting the identity (18) into formula (17) we get the integral representation of the Jacobian

$$\begin{aligned} J(\bar{Q}, \vec{m}) &= \int dz \exp\left[-2i \sum_k' (\bar{C}_k \bar{p}_k + \bar{S}_k \bar{q}_k) \right. \\ &\quad \left. + \sum_{n=2}^{\infty} \frac{i^n}{n!} V_n(\vec{z} \cdot \vec{m})\right] \end{aligned} \quad (20)$$

with $V_n(\vec{z} \cdot \vec{m}) = \sum_{j=1}^N \omega_n(\vec{z} \cdot \vec{m}_j)$. Now, having inserted the integral representation (20) into formula (14) and taken the Gaussian integral on dQ measure, we get the integral representation for the replicated partition function, our starting point:

$$\begin{aligned} \overline{\hat{Z}_N^s} &= \exp\left\{s \cdot \sum_k' \left[\nu_k + \ln\left(\frac{\pi}{\nu_k}\right)\right]\right\} \cdot \text{Tr}_N^K \\ &\quad \times \left[\int dz \exp\left(-\sum_k' \frac{\vec{z}_k \cdot \vec{z}_{-k}}{\nu_k} + \sum_{n=2}^{\infty} \frac{i^n}{n!} V_n(\vec{z} \cdot \vec{m})\right) \right]. \end{aligned} \quad (21)$$

When going from the initial expression (5) for the replicated partition function to the final one (21) we have used the way via the Jacobian integral representation (20) different from

other approaches.^{17,23,24} This way makes all calculations for the free energy, DOSE, and the OSE correlators to be of the same type.

C. RPA for $F_N(\beta)$

From now on we confine ourselves to the case $K=1/2$, for which the electroneutrality condition (3) does not have to be taken into account specifically.²⁵ The RPA corresponds to $V_n=0$ for all $n \geq 3$. Having inserted Ising spins (4) into V_2 from Eq. (20), we get

$$V_2(\vec{z}, \vec{m}) = \sum_k' (\vec{z}_k, D\vec{z}_{-k}), \quad D^{a,b} = \frac{1}{N} \cdot \sum_{j=1}^N \sigma_j^a \sigma_j^b. \quad (22)$$

So, D is the matrix in a s -dimensional replica space. Having taken Gaussian integrals in the formula (21) (with $V_n=0$ for $n \geq 3$) and transforming the determinants arising into exponential form, we get, after some simple algebra,

$$\begin{aligned} \overline{\hat{Z}_N} &= \exp\left(s \cdot \sum_k' [\nu_k - \ln(1 + \nu_k)]\right) \cdot \text{Tr}_N \\ &\times \left[\exp\left(N \sum_{n \geq 2} \frac{(-1)^n}{n} \cdot \gamma_n \cdot \text{Sp}(\check{D}^n)\right) \right] \quad (23) \end{aligned}$$

with $D = 1 + \check{D}$, Sp as the trace in the replica space, and with g_k and γ_n defined as

$$g_k = \left(\frac{\nu_k}{1 + \nu_k}\right), \quad \gamma_n = \frac{1}{N} \left(\sum_k' g_k^n\right), \quad n \geq 2. \quad (24)$$

The symbol Tr_N in Eq. (23) means the trace without the restrictions due to the electroneutrality condition (3). Note that all γ_n entering Eq. (23) allow for going to the limits $\Lambda \rightarrow \infty$, $\alpha \rightarrow 0$. It is shown below that $\text{Tr}_N[\dots]$ entering Eq. (23) equals to $\exp[N \ln 2 + O(1)]$, where $O(1)$ is the order of the corresponding term at $N \rightarrow \infty$. So, from Eq. (23) we get immediately in the leading order on N : $\beta F_N/N = -\ln 2 + (1/N) \sum_k' [\ln(1 + \nu_k) - \nu_k]$. This expression is the special case of the common formula (we have returned to natural dimensions in this case)

$$\beta F_N/V = -n \left[K \ln\left(\frac{1}{K}\right) + L \ln\left(\frac{1}{L}\right) \right] - k_d^3/12\pi \quad (25)$$

which helps us to understand the meaning of two terms entering it. Since at high temperatures each of the N donor sites is ionized with probability K and is neutral with probability L , the first term in Eq. (25) is nothing but the entropy density ascribed to the sites in the unit volume. The second term is the Debye correction to the free energy of the electrolyte²⁸ with the effective ionic force $f = e^2 n K L$ and the radius of the Debye screening $r_d = k_d^{-1} = (4\pi\beta f)^{-1/2}$. In Fig. 1 the energy $e(T)$ per site found from the formula (25) is compared with the data of MC simulations. The deviation between the MC data and the theoretical predictions, seen in the high-temperature region, has the natural explanation in growing size influence with increasing temperature, the screening ra-

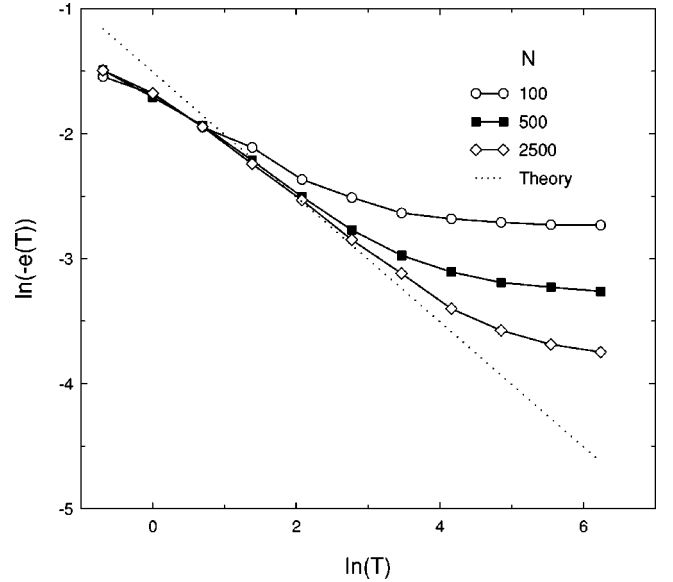


FIG. 1. Energy $e(T)$ per one site vs temperature T for the case $K=0.5$. MC simulations with the periodic boundary conditions were made with averaging on five specimen of each N : 100, 500, 2500. Statistical errors of the averaging on MC chains are less than the symbol sizes. The theoretical formula $e(T) = -\sqrt{\pi/T} \cdot (K \cdot L)^{3/2}$ was found from Eq. (25) of the text via the Gibbs rule.

dius $r_d \sim \sqrt{T}$ being comparable to the specimen size. As is seen from Fig. 1, at a given temperature the deviations mentioned decrease with increasing N . Thus it follows from this comparison that the theoretical results are in good quantitative agreement with the MC data in the temperature region (1). In conclusion, we shortly discuss the method to estimate, in the limit $N \rightarrow \infty$, orders of terms, arising as the result of expanding the exponent entering formula (23) under trace sign. The method will be illustrated by the example²⁹ $\Lambda_2 = \text{Tr}_N\{\exp[-(N\gamma_2/2)\text{Sp}(\check{D}^2)]\}$. By developing the exponent in powers of $N\text{Sp}(\check{D}^2)$ we will have to deal with sums (on the sites i, j, \dots and the replica indices a, b, \dots) of the monos, i.e., products of Ising spins σ_j^a . Such a mono gives a nonzero contribution, after Tr_N has been taken, only if each spin σ_j^a enters into it with an *even* power. Since the matrix \check{D} has the zero diagonal elements in replica space and only *one* sum on the site indices [see Eq. (22)] such an even power of σ_j^a can only arise in that case when, as the minimum, two terms belonging to the *different* \check{D} matrices have the index j as common. Because each \check{D} has the factor $(1/N)$ [see Eq. (22)] these coincidences considerably reduce the power of N in the mono contribution. Using this method, we have estimated the orders of all terms $\text{Tr}_N\{[N\text{Sp}(\check{D}^2)]^p\}$ with $p = 0, 1, 2, \dots$ and found that each of them has to be of the order $O(1)$, at $N \rightarrow \infty$, except the one with $p=0$. The $p=0$ case gives the result 2^{Ns} which has been used in the expression for F_N . We have estimated, too, contributions from the terms $n \geq 3$ entering the exponent of Eq. (23) and shown that all they are of the order $O(1/N)$ at $N \rightarrow \infty$.

III. RPA FOR G

It is convenient to deal with $G(\varepsilon)$, defined through $g(\varepsilon)$, by the relation $g(\varepsilon) = \beta \cdot G(\beta\varepsilon)$, and with $\hat{e}_j = \beta \cdot \hat{\varepsilon}_j$ instead of OSE being defined⁴ as $\hat{\varepsilon}_j = \delta\hat{H}_N / \delta m_j$. Having taken the derivative $\delta / \delta m_j$ of the energy (2) and used the definition (8) for CV's and the expansion (10) for the Coulomb potential, we get

$$\hat{e}_j = (1/\sqrt{NKL}) \cdot \sum_{k \neq 0} \nu_k \cdot \hat{Q}_{-k} \exp(ik\vec{x}_j) - (m_j/NKL) \cdot \sum_{k \neq 0} \nu_k. \quad (26)$$

The main object of our interest,

$$\overline{[e^{i\omega\hat{e}_j}]_T} = \lim_{s \rightarrow 0} \text{Tr}_N \left[e^{i\omega\hat{e}_j(m_c)} \cdot \prod_{a=1}^s e^{-\beta\hat{H}_N(m_a)} \right], \quad (27)$$

is related to $G(e)$ via the Fourier transform

$$G(e) = \overline{[\delta(e - \hat{e}_j)]_T} = \int \frac{d\omega}{2\pi} e^{-i\omega e} \overline{[\exp(i\omega\hat{e}_j)]_T}. \quad (28)$$

The c index in the formula (27) has been used to mark that one out of all replicas to which \hat{e}_j belongs. To switch in formula (27) to CV's the technique already described in Sec. II was used. Omitting details, we present here only the final result for the case $K=1/2$ in RPA:

$$\begin{aligned} \overline{[e^{i\omega\hat{e}_j}]_T} &= \lim_{s \rightarrow 0} \exp \left[s \cdot \sum_k' [\nu_k + \ln(\pi/\nu_k)] - (4\omega^2/N) \right. \\ &\quad \times \left(\sum_k' \nu_k \right) \left. \right] \cdot \text{Tr}_N \left(\prod_k' [\pi^s \cdot \det \Gamma_j(k)]^{-1} \right. \\ &\quad \left. \times \exp \{ -[\vec{A}_j, \Gamma_j^{-1}(k)\vec{A}_j] - (4i\omega/N)\nu_k \cdot \sigma_j^c \} \right) \end{aligned} \quad (29)$$

with

$$\Gamma_j^{a,b} = (\delta_{a,b}/\nu_k + D_j^{a,b}), \quad D_j^{a,b} = \sum_{l \neq j} \sigma_l^a \cdot \sigma_l^b, \quad (30)$$

$$\vec{A}_j = (2/\sqrt{N})(i\omega \cdot \vec{e}_c - \vec{\sigma}_j/2), \quad \vec{e}_c = [\delta_{c,a}]_{a=1}^s. \quad (31)$$

The following transformations aim to extract and then exclude the terms of order $O(1/N)$ in the thermodynamic limit:

$$\begin{aligned} \prod_k' [\pi^s \det \Gamma_j(k)]^{-1} &= \exp \left[s \cdot \sum_k' [\ln(\nu_k/\pi) - \ln(1 + \nu_k)] \right. \\ &\quad \left. + s \cdot \left(\frac{1}{N} \sum_k' g_k \right) + \frac{1}{2} \gamma_2 N \text{Sp}(\check{D}_j^2) \right], \end{aligned} \quad (32)$$

$$\sum_k' [\vec{A}_j, \Gamma(k)_j^{-1} \vec{A}_j] = \left(\frac{4}{N} \sum_k' g_k \right) \cdot \left(-\omega^2 + \frac{1}{4}s - i\omega\sigma_j^c \right). \quad (33)$$

As in Eq. (29) so in Eq. (32) is the series present which becomes divergent after taking the regularization out. However, inserting the expressions (32) and (33) into Eq. (29) gets the mutual compensation of these divergences, and we get the result

$$\begin{aligned} \overline{[e^{i\omega\hat{e}_j}]_T} &= \lim_{s \rightarrow 0} \exp \left(s \cdot \sum_k' [\ln(1 + \nu_k) - \nu_k] \right. \\ &\quad \left. - \gamma_1 \omega^2 \right) \cdot \text{Tr}_N \left[\exp \left(\frac{1}{2} N \gamma_2 \cdot \text{Sp}(\check{D}_j^2) - i\gamma_1 \omega \sigma_j^c \right) \right] \end{aligned} \quad (34)$$

remaining finite after removing the regularization, with γ_1 being defined as

$$\gamma_1 = (4/N) \sum_k' (\nu_k - g_k) = (4/N) \sum_k' \left(\frac{\nu_k^2}{1 + \nu_k^2} \right) = \frac{1}{2} \left(\frac{\pi}{T^3} \right)^{1/2}. \quad (35)$$

Since \check{D}_j does not depend on $\vec{\sigma}_j$, the Tr_j on the $\vec{\sigma}_j$ together with the $\exp(-i\gamma_1\omega\sigma_j^c)$ can be taken out of the brackets in Eq. (34). The trace Tr_N on the rest terms, already calculated in Sec. II, gets the result $\exp[s \cdot N \ln 2 + s \cdot O(1)]$. With the first exponent in Eq. (34), depending on s , it gives the free energy found in RPA up to order $O(1)$, so we have

$$\begin{aligned} \overline{[e^{i\omega\hat{e}_j}]_T} &= \lim_{s \rightarrow 0} \{ \exp(-s \cdot \beta \cdot F_N^{RPA} - \gamma_1 \omega^2) \cdot \text{Tr}_j [e^{i\gamma_1 \omega \sigma_j^c}] \} \\ &= e^{-\gamma_1 \omega^2} \cdot \cos(\gamma_1 \omega). \end{aligned} \quad (36)$$

Then $G(e)$ is found by insertion of Eq. (36) into Eq. (28). For DOSE $g(\varepsilon)$ we have then

$$\begin{aligned} g(\varepsilon) &= \frac{1}{4\sqrt{\pi\lambda T^{1/2}}} \left[\exp \left(-\frac{(\lambda/T^{1/2} - \varepsilon)^2}{4\lambda T^{1/2}} \right) \right. \\ &\quad \left. + \exp \left(-\frac{(\lambda/T^{1/2} + \varepsilon)^2}{4\lambda T^{1/2}} \right) \right], \quad \lambda = \sqrt{\pi}/2. \end{aligned} \quad (37)$$

In region (1) $g(\varepsilon)$ has a cupola shape with its center at $\varepsilon = 0$. With decreasing of the temperature the depletion of DOSE shape in the center $\varepsilon = 0$ rises starting with the temperature $(\pi/16)^{1/3}$. This depletion would be considered as the start of the Coulomb correlation gap if the RPA were applicable below this temperature. To compare our result (37) to MC data we were forced to run simulations with specimens of large N . Matrices of intersite Coulomb interactions did not get into access memory, so lengths of MC chains were comparatively short. As is seen from Fig. 2, the RPA is in the

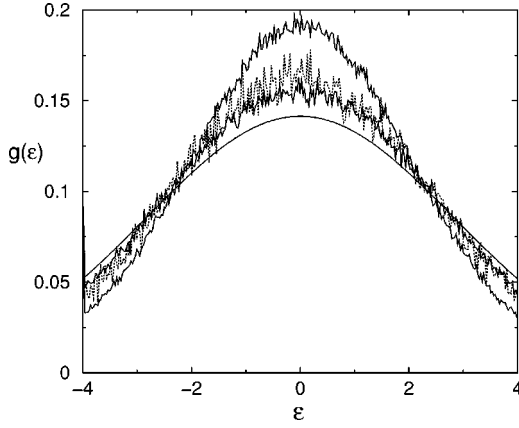


FIG. 2. The shape of the DOSE, $g(\varepsilon)$, for the case of $K=0.5$ and $T=10$. MC simulations with the periodic boundary conditions were made for one specimen of each N : 500, 2500, 12 500, 62 500. The MC curves have diminishing height of maxima with increasing N . The last two ($N=12500$ and $N=62500$) merge. The formula (37) of the text was for full down curve.

qualitative agreement with the MC data at $T=10$, provided the specimen size is large enough. Nevertheless, even at $T=10$ a small quantitative deviation exists between theory and MC experiment. This disagreement was shown to decrease with increasing temperature. In the temperature range $10 > T > 1$ the RPA results remain in qualitative agreement with MC data, but the deviations are then not explained by too small specimen sizes and grow with decreasing temperature. In this temperature range, as we believe, the high-temperature corrections to RPA similar to those known from the classical plasma theory²⁴ could have improved the comparison to MC simulations. In the low-temperature region, $T < 1$, RPA does not correctly describe the DOSE behavior even on a qualitative level.

IV. OSE CORRELATIONS

Here we define the pair OSE correlator $g(\varepsilon_1, \varepsilon_2, r)$ and calculate it in the RPA. As in the case of $g(\varepsilon)$, it is convenient to work with $\hat{e}_j = \beta \cdot \varepsilon_j$ and with $G(e_1, e_2, r)$ defined via the relation $g(\varepsilon_1, \varepsilon_2, r) = \beta^2 \cdot G(\beta \varepsilon_1, \beta \varepsilon_2, r)$.

A. Definition of $g(\varepsilon_1, \varepsilon_2, r)$

For a given specimen \mathbf{R} and charge distribution $[m_j]_1^N$ let us consider the number of sites from the total set $[2 \leq j \leq N]$ being in the spherical layer $(r, r+dr)$ around the site $j=1$ and with energies \hat{e}_j from the strip (e_2, e_2+de_2) , provided the site $j=1$ has its energy in (e_1, e_1+de_1) .

Evidently, this number is $\sum_{j=2}^N \delta(\hat{e}_1 - e_1) \delta(\hat{e}_j - e_2) \delta(r_{1,j} - r) de_1 de_2 dr$. Having averaged this number over the thermal equilibrium and the distributions of the sites $[2 \leq j \leq N]$, we define the correlator by the relation

$$(N-1) \cdot \overline{\{[\delta(\hat{e}_1 - e_1) \delta(\hat{e}_2 - e_2) \delta(r_{1,2} - r)]\}_T}^N de_1 de_2 dr = 4\pi r^2 \left(\frac{N-1}{V} \right) \cdot G(e_1, e_2, r) de_1 de_2 dr. \quad (38)$$

The left-hand side of Eq. (38) is this number averaged over the thermal equilibrium and the positions of all sites but the first one. It follows from the definition (38) that $G(e_1, e_2, r)$ is the probability density to find one out of $(N-1)$ sites with energy in the interval (e_2, e_2+de_2) and being placed in the spherical layer $(r, r+dr)$ around a given site $j=1$ provided the energy of given site is in the interval (e_1, e_1+de_1) . Since the left-hand side of Eq. (38) does not depend on the first site position, averaging on the position of this site does not change the definition (38). So we can finally define $G(e_1, e_2, r)$ by the following relation:

$$\overline{[\delta(\hat{e}_1 - e_1) \delta(\hat{e}_2 - e_2) \delta(r_{1,2} - r)]_T} = \left(\frac{4\pi r^2}{V} \right) \cdot G(e_1, e_2, r). \quad (39)$$

From this last definition the symmetry of G with respect to the transposition of its energy variables is evident. Because the energies \hat{e}_1, \hat{e}_2 depend on \mathbf{R} only through the mutual site distances we have the identity

$$\overline{[\delta(\hat{e}_1 - e_1) \delta(r_{1,2} - r)]_T} = \left(\frac{4\pi r^2}{V} \right) \cdot G(e_1). \quad (40)$$

It follows from Eq. (39) and (40) that $G(e_1, e_2, r)$ is related to $G(e_1)$ through the self-consistency conditions

$$\int G(e_1, e_2, r) de_2 = G(e_1), \quad \int G(e_1, e_2, r) de_1 de_2 = 1. \quad (41)$$

If we expect the decoupling of correlations takes place at large r the formula for this decoupling being in the correspondence with the self-consistency conditions (41) has the form

$$G(e_1, e_2, \infty) = G(e_1) \cdot G(e_2). \quad (42)$$

Our RPA results will be shown to obey the decoupling condition (42). As for the case of $G(e)$, all calculations are convenient to do with the Fourier transform \tilde{G} of the correlator entering Eq. (39). What we actually calculate is the replicated form of this \tilde{G} ,

$$\left(\frac{4\pi r^2}{V} \right) \cdot \tilde{G}(\omega_1, \omega_2, r) = \lim_{s \rightarrow 0} \text{Tr}_N \left[\delta(r_{1,2} - r) \exp \left(\sum_{\alpha=1}^2 i \omega_\alpha \cdot \sigma_\alpha^c - \beta \sum_{a=1}^s \hat{H}_N(m_a) \right) \right]. \quad (43)$$

B. RPA for $G(e_1, e_2, r)$

Switching to CV's in the formula (43) is quite analogous to the cases of DOSE and the replicated partition function, so we only present here the final result for $K=1/2$ in RPA:

$$\begin{aligned} \left(\frac{4\pi r^2}{V}\right) \tilde{G}(\omega_1, \omega_2, r) = \lim_{s \rightarrow 0} e^Q \cdot \int \int \frac{\delta(r_{1,2}^y - r)}{V^2} d\vec{y}_1 d\vec{y}_2 \text{Tr}_N \left(\left\{ \exp \left[\left(\frac{4i}{N} \right) \left(\sum_{\alpha=1}^2 \omega_\alpha \sigma_\alpha^c \right) \cdot \left(\sum_k' \nu_k \right) \right] \cdot \left[\prod_k' \int \frac{d\vec{p}_k}{\pi^s} \right. \right. \right. \\ \times \exp \left(-(\vec{p}_k, \Gamma_k \vec{p}_k) - 2i \sum_{\alpha=1}^2 (\vec{p}_k, \vec{A}_\alpha) \cdot \cos(\vec{k} \vec{y}_\alpha) \right) \left. \right] \cdot \left[\prod_k' \int \frac{d\vec{q}_k}{\pi^s} \right. \\ \left. \left. \left. \times \exp \left(-(\vec{q}_k, \Gamma_k \vec{q}_k) - 2i \sum_{\alpha=1}^2 (\vec{q}_k, \vec{A}_\alpha) \cdot \sin(\vec{k} \vec{y}_\alpha) \right) \right] \right] \right\} \end{aligned} \quad (44)$$

with

$$\begin{aligned} Q = s \cdot \sum_k' [\nu_k + \ln(\pi/\nu_k)] - 4\omega_1 \omega_2 \Phi_c(r) - 4(\omega_1^2 + \omega_2^2) \cdot \left(\frac{1}{N} \sum_k' \nu_k \right), \\ \vec{A}_\alpha = (2/\sqrt{N}) \cdot \left(i\omega_\alpha \vec{e}^c - \frac{1}{2} \vec{\sigma}_\alpha \right), \quad \alpha = 1, 2, \\ \Gamma_k^{a,b} = (\delta_{a,b}/\nu_k + D_{a,b}^{(2)}), \quad D_{a,b}^{(2)} = \left(\frac{1}{N} \right) \cdot \sum_{j=3}^N \sigma_j^a \sigma_j^b. \end{aligned} \quad (45)$$

Note that $D^{(2)}$ does not depend on $\vec{\sigma}_{1,2}$ and therefore the calculations with $D^{(2)}$ can be done at the constant replicated spins $\vec{\sigma}_{1,2}$. The following transformation of Eq. (44) consists of taking Gaussian integrals and selecting those terms from arising determinants which survive in the thermodynamic limit, $N \rightarrow \infty$. The algebra is simple but cumbersome, so we present here only the final result of the manipulations mentioned:

$$\begin{aligned} \tilde{G}(\omega_1, \omega_2, r) = \exp[-2\omega_1 \cdot \omega_2 \cdot \Phi_p(r) - (\omega_1^2 + \omega_2^2) \cdot \Phi_p(0)] \cdot \left(\frac{\cos\{(\omega_1 + \omega_2) \cdot [\Phi_d(r) - \Phi_p(0)]\}}{1 + \exp[\Phi_d(r)]} \right. \\ \left. + \frac{\cos\{(\omega_1 - \omega_2) \cdot [\Phi_d(r) + \Phi_p(0)]\}}{1 + \exp[-\Phi_d(r)]} \right), \end{aligned} \quad (46)$$

where the potentials $\Phi_p(r)$ and $\Phi_d(r)$ are defined as

$$\begin{aligned} \Phi_p(r) = \left(\frac{4}{N} \right) \sum_k' \left(\frac{\nu_k^2}{1 + \nu_k} \right) \cdot \cos(\vec{k} \vec{r}) = \left(\frac{\pi}{4T^3} \right)^{1/2} \cdot \left(\frac{1 - e^{-\alpha}}{\alpha} \right), \\ \Phi_d(r) = \left(\frac{4}{N} \right) \sum_k' \left(\frac{\nu_k}{1 + \nu_k} \right) \cdot \cos(\vec{k} \vec{r}) = (k_d^2/2\pi r) \cdot e^{-\alpha} \end{aligned} \quad (47)$$

with $\alpha = (k_d \cdot r)$ and $k_d^2 = (\pi/T)$. It is seen that $\Phi_d(r)$ is proportional to the Coulomb potential screened with Debye radius r_d . In the screening region ($\alpha > 1$) we can neglect $\Phi_d(r)$ in comparison to $\Phi_p(r)$ because the latter behaves as the unscreened Coulomb potential. We consider here the asymptotical behavior in the region $\alpha > 1$. Aiming to compare our results with those of Blanter and Raikh¹⁶ we consider in detail only the cases of $(e_1, e_2): (e, e), (e, -e)$ and $(0, e)$.

C. $e^{-\alpha} = 0$ approximation for G

In this approximation we have $\Phi_d(r) = 0, \Phi_p(r) = \gamma_0 \cdot x$, where $\gamma_0 = (\pi/4T^3)^{1/2}$ and $x = 1/\alpha$. The three above mentioned special cases are

$$\begin{aligned} G(e, \pm e, r) = \frac{1}{16\pi \gamma_0 \sqrt{1-x^2}} \cdot \left[\exp \left(-\frac{\gamma_0 \cdot (1+y)^2}{2(1 \pm x)} \right) \right. \\ \left. + \exp \left(-\frac{\gamma_0 \cdot (1-y)^2}{2(1 \pm x)} \right) \right. \\ \left. + 2 \cdot \exp \left(-\frac{\gamma_0 \cdot y^2}{2(1 \pm x)} - \frac{\gamma_0}{2(1 \mp x)} \right) \right], \end{aligned} \quad (48)$$

$$\begin{aligned} G(0, e, r) = \frac{\exp \left(-\frac{e^2}{4\gamma_0 \cdot (1-x^2)} \right)}{16\pi \gamma_0 \sqrt{1-x^2}} \cdot \left[\exp \left(-\frac{e + \gamma_0}{2(1+x)} \right) \right. \\ \left. + \exp \left(-\frac{\gamma_0 - e}{2(1+x)} \right) + \exp \left(-\frac{\gamma_0 + e}{2(1-x)} \right) \right. \\ \left. + \exp \left(-\frac{\gamma_0 - e}{2(1-x)} \right) \right]. \end{aligned} \quad (49)$$

In formula (48) we have used the variable $y: e = \gamma_0 \cdot y$. By taking $x=0$ in the formulas (48) and (49) it is easily seen

that the decoupling relations (42) are fulfilled in all cases considered. Developing in small x in Eq. (48), with $y = O(1)$, we get

$$\frac{G(e, \pm e, r)}{G(e, \pm e, \infty)} = 1 \pm (\gamma_0 x/2) \cdot [y - \tanh(\gamma_0 y/2)]^2 + O(x^2). \quad (50)$$

The development (48) in small x and y up to second order in x gives

$$\frac{G(e, \pm e, r)}{G(e, \pm e, \infty)} = 1 \pm \frac{\gamma_0 \cdot x}{2} \cdot y^2 \left(1 - \frac{\gamma_0}{2}\right)^2 + x^2 \cdot \left(\frac{1}{2} - \frac{\gamma_0}{2} + \frac{\gamma_0^2}{8}\right). \quad (51)$$

As it follows from Eq. (51), in the “low-energy” region $\gamma_0 \cdot y^2 < x$ we have attractive correlations proportional to x^2 whereas in the rest of the region, $\gamma_0 \cdot y^2 > x$, decoupling obeys the law (50) depending on $\text{sgn}(e_1 \cdot e_2)$ and proportional to x .

In summary, in terms of natural parameters the asymptotic correlation behavior is as follows. The condition (1) of RPA applicability together with one for the screening regime [$x < 1$ and $y = O(1)$] can be expressed as $1 < T < \pi \cdot r^2$, $\varepsilon^2 \sim \pi/T$ and the low-energy regime corresponds to $\varepsilon^2 < T/2r$. Note that in the case that both of these conditions are fulfilled, the inequality $(T/\pi)^{1/2} < r < T^2/2\pi$ has to be valid. In this region the correlators (48) obey the attractive law $\sim T/\pi r^2$. The “high-energy” region, where the inequality $r > T^2/2\pi$ is fulfilled, corresponds to $r > T^2/2\pi$. In this region the asymptotic behavior (50) works and decoupling obeys the law $\sim \text{sgn}(\varepsilon_1 \cdot \varepsilon_2) \cdot (T/\pi)^{1/2} \cdot (1/r)$. To investigate the asymptotic behavior of $G(0, e, r)$ at $x \rightarrow 0, y = O(1)$ we have developed formula (49) in powers of small x , assuming $e = O(1)$:

$$\frac{G(0, e, r)}{G(0, e, \infty)} = 1 - x^2 \cdot \left[\frac{e^2}{4\gamma_0} + \frac{e^2}{8} + \frac{\gamma_0 \cdot e}{4} \cdot \tanh\left(\frac{e}{2}\right) - \frac{1}{2} + \frac{\gamma_0}{2} - \frac{\gamma_0^2}{8} \right]. \quad (52)$$

It follows from Eq. (52) that for $e > 1$ (i.e., $\varepsilon > T$) a correlation repulsion obeying the law $\sim T/r^2$ takes place and with diminishing e this repulsion slowly goes over into attractive correlation characteristic to the low energy region.

V. DISCUSSION

To what extent do the results found depend on the model? Specifically, does the decoupling of the OSE correlations depend on the features of the model considered? In Ref. 16, the only one we were able to find on this subject, the DOSE and the OSE pair correlators have been calculated from self-consistent equations (see the discussion in Sec. I) for the two-dimensional case and for pair potentials $V(r)$, without singularities at $r=0$ and decreasing no slower than $1/r^2$ as $r \rightarrow \infty$. So, any comparison of our results to those of Ref. 16 inevitably has to be of a qualitative character, even in the region $V(r)/T < 1$ where RPA is assumed to be applicable.

The comparison of the formulas (29)–(33) of Ref. 16 to our Eq. (37) for DOSE does not confirm the functional form $g(\varepsilon) \sim f(\varepsilon/T)$ of the temperature dependence found in Ref. 16. Our formula (51), taken at $e=0$, shows attractive correlations decoupling via $\sim T/r^2$ whereas the formula (43) of Ref. 16 shows attractive decoupling $\sim V(r)/T$. In our case the asymptotic behavior at $\varepsilon \sim T$ gives a decoupling of the repulsive type $\sim \sqrt{T} \cdot \varepsilon^2/r^2$ whereas the decoupling found from the formula¹⁶ (47) is repulsive, as well, but with a different temperature dependence: $\sim V^2(r)/T^2$. It would be very interesting to solve the equations¹⁶ in the high-temperature region (1) for the three-dimensional case and with Coulomb pair interaction as $V(r)$ in order to compare to our results.

VI. CONCLUSION

In this section we use natural dimensions for all variables considered. We have considered in RPA a Coulomb glass model with randomly distributed donor sites and with acceptor charges equally smeared on donors, $-K \cdot e$ on each. Our results for the energy and DOSE were shown to be in good agreement with MC simulation data in the temperature region $T > e^2 \cdot n^{1/3}$. In this region the thermodynamics of the Coulomb glass model is similar to the one for an electrolyte in the Debye screening regime with screening radius $r_d = (T/\pi e^2 n)^{1/2}$. We have investigated the behavior of the OSE correlator $g(\varepsilon_1, \varepsilon_2, r)$ in the asymptotic regime $r > r_d$: the cases $g(\varepsilon, \pm \varepsilon, r)$ were considered at the energy scale $\varepsilon^2 \sim (n \cdot e^6/T)$. We have shown that in the low-energy region, where the inequality $(T/e^2 n^{1/3})^{1/2} < r \cdot n^{1/3} < (T/4\pi^2 e^2 n^{1/3})^2$ fulfills, the attractive correlation exists between sites decreasing according to the law $\sim (T/n e^2 r^2)$. In the region, where $r \cdot n^{1/3} > (T/4\pi^2 e^2 n^{1/3})^2$, this decoupling changes into the regime obeying the new law $\sim \text{sgn}(\varepsilon_1 \cdot \varepsilon_2) (T/e^2 r)$. The repulsion between sites with OSE of different signs of $(\varepsilon - \mu)$ is well known since the early theories^{2–4} treating the Coulomb gap phenomena at $T=0$. The attractive correlations between sites of the same $\text{sgn}(\varepsilon - \mu)$ were noted in the narrow energy strip near the Fermi level μ in the simulations of Davies, Lee, and Rice²⁷ made at $T=0$. The main result of our work is that even in the temperature region, where the thermodynamics of a Coulomb glass is mainly determined by the Debye screening effects, unscreened correlations of long-range nature still exist between OSE’s. Because a similarity takes place between the OSE correlations found in our investigation and those²⁷ for $T=0$ we believe that our results would shed some light on the structure of the low-temperature states of Coulomb glasses.

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