Ion correlations and ion microfields at impurities in dense plasmas

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An impurity placed in a plasma modifies the particle-particle correlations in the plasma. This impurity-plasma-plasma correction is relevant to ion-microfield calculations in hot dense plasmas as well as to models of the fractional quantum Hall excitations in terms of impurity-plasma systems. We show how to calculate such impurity-plasma-plasma corrections and apply them to a calculation of the Baranger-Mozer (BM) second-order microfield at He, Li, Be, and B impurities in a hydrogen plasma. Such a calculation for a dense plasma requires a definition of the electric field at the impurity due to an individual plasma ion in the plasma. We show how the traditional uniform jellium background assumption can be transcended via a deconvolution of the electron density obtained from a density-functional calculation for the plasma that incorporates the fully self-consistent nonlinear screening effects. Finally we carry out all-order resummations of the BM series beyond second order using the weighted-chain-sum method and also two models of the adjustable parameter exponential approximation.

I. INTRODUCTION

The electronic energy levels of an ion placed in a plasma become broadened and shifted due to the constantly varying potential arising from the changing ion configuration of the plasma medium. The concept of the ion microfield,[1] that is, the electric field produced at the site of the radiator by the perturber ions, has been introduced to model this problem in a relatively simple fashion and has been of great value in the theory of spectral line broadening. Ion microfields can be useful in a number of other related problems[2] if the ion microfield refers to the actual electric field at the "radiator ion" (impurity ion) rather that to a "field" defined in a less physical manner.

Usually the term "strong coupling" is taken to mean strong ion-ion coupling, but the electron-ion coupling is assumed to be weak. However, in this paper "strong coupling" applies to the electron-ion interaction as well and hence the possibility of the formation of bound states (ions with structure) has to be considered from the outset. In this paper we specifically treat cases where there is strong electron-ion coupling between the electrons of the plasma and the radiator ion, while the ion-ion coupling in the plasma is relatively weak ($\Gamma < 1$).

Working within the Baranger-Mozer (BM) cluster expansion[3] for the ion microfield we showed in previous papers[4,5] that density-functional theory (DFT) can be used to avoid the weak electron-ion coupling assumption inherent in many previous calculations of ion microfields. This enabled us to treat situations involving bound states and arbitrary electron degeneracies. In effect, instead of the "weak-coupling" approach where it is assumed that the determination of the microfields is essentially a problem in statistical mechanics divorced from the problem of defining the single-particle states and correlation functions of the radiator and perturber system, we emphasize the need for a unified approach, especially for regimes outside weakly coupled plasmas, since the statistical mechanics of the ion correlations and the evaluation of the various traces cannot be separated from each other. The density-functional theory of plasmas provides such a unified approach when associated with the Baranger-Mozer expansions which can be partially resummed[5] to all orders using a weighted-chain-sum (WCS) approximation or an adjustable parameter exponential approximation (APEX) model.[6]

Our use of the BM expansion and the WCS approximation depends on a Kirkwood-type decomposition of the impurity-plasma-plasma triplet distribution function $g_{ipp}(0,1,2)$ for an impurity ion at the origin $\mathbf{r}_0$, and two perturber ions (plasma ions) at $\mathbf{r}_1$ and $\mathbf{r}_2$. That is, it is assumed that the triplet distribution can be replaced by a product of pair distributions:

$$g_{ipp}(0,1,2)=g_{ip}(0,1)g_{ip}(0,2)g_{pp}(1,2)\ . \tag{1.1}$$

Further, $g_{pp}(1,2)$ was taken to be $g^0_{pp}(|\mathbf{r}_1-\mathbf{r}_2|)$, i.e., the pair distribution function (PDF) of the homogeneous plasma (no impurity ion at the origin). The PDF's needed in (1.1) were then calculated using DFT.[7] This type of approximation is rather common in various plasma problems and is generally thought to be valid for moderate to weak ion-ion coupling regimes. The objective of this paper is to investigate the effect of strong electron-radiator coupling rather than to improve the Kirkwood decomposition which is expected to be good for the ion-ion coupling regimes ($\Gamma < 1$) studied here.

A principal objective of the present paper is to improve on (1.1) by including the effect of the impurity ion on g_{pp}.

That is, we retain the product form but replace (1.1) by

$$g_{ipp}(0,1,2)=g_{ip}(0,1)g_{ip}(0,2)g_{pp}(1,2|r_0)\ , \tag{1.2}$$

where $g_{pp}(1,2|r_0)$ is a plasma-plasma pair distribution function which takes account of the presence of the impurity ion at the origin $\mathbf{r}_0$ and defined by (1.2). The correlations contained in g_{pp} are probably similar to what Iglesias and Hooper[8] have called "noncentral" correlations. The difference

$$\Delta h(1,2|r_0)=g_{pp}(1,2|r_0)-g^0_{pp}(1,2)\ , \tag{1.3}$$

where $g^0_{pp}(1,2)=g^0_{pp}(|\mathbf{r}_1-\mathbf{r}_2|)$ is the homogeneous pair distribution function, will be called the impurity-plasma-plasma correlation correction (*ipp* correction). Although these types of corrections have usually been neglected, they are frequently as important as the corrections obtained by all-order summations of the BM series and need to be considered, especially for charged impurities. The idea of retaining the product form (1.1) with modified pair functions has also been examined in the context of the triplet correlations[9] of the pure homogeneous plasma. The present problem of calculating the *ipp* correction has been central to the evaluation of the excitation energies in fractional quantum Hall (FQH) systems.[10,11] The present paper will clarify some obscure aspects and possible inconsistencies in the plasma mapping of the FQH-impurity problem. We have carried out explicit calculations of the *ipp* correction to the ion microfields at He, Li, B, and Be impurities in a hydrogen plasma, to expose the effects of modifications in the "noncentral" correlations (*ipp* correction).

A second objective of this study is to discuss how the effective electric field at the radiator should be calculated when linear response is no longer applicable, and when there is a significant difficulty in assigning a specific effective ionic charge Z to the ions in the plasma. Iglesias and Dufty,[12] (also Dufty[1]) have emphasized that the electric field to be used in a given microfield calculation depends on the "microfield formalism" used. For example, it depends on whether electron fields as well as ion fields are included, and on how ion screening and electron screening are treated. In a strongly coupled system even the definitions of the quasi-independent "perturber atoms," ions, etc., require careful consideration. These determine the mean charge $\bar{Z}$, the screening charges, the Debye fields or the more accurately calculated (i.e., beyond the linear-response approximation inherent in Debye theory) *physical* electric fields. These in turn should *in principle* modify the level structure and induce fluctuations in Z, requiring a self-consistent determination of the atomic physics, continuous spectrum, pair-correlation functions, and the microfields of the coupled system, i.e., impurity and plasma. Hence we believe that, in a practical sense, the clearest physical picture is obtained if microfields are calculated using the best possible approximation to the *physical* electric fields generated from the electron-screened ions. As such we shall discuss carefully how the screened fields are to be calculated, without making the approximation of uniform jellium backgrounds. Such electric fields would be useful in the calculation of other physical properties[2] as well.

The plan of the paper is as follows. In Sec. II we review the Baranger-Mozer cluster expansion and the WCS all-order approximation pointing out how the *ipp* corrections enter into the theory. Then we consider the evaluation of the *ipp* corrections via (i) a two-component plasma (TCP) model made up of impurity ions and plasma ions, and (ii) an inhomogeneous plasma (IHP) model where the effect of the impurity ion is treated as an external potential. In Sec. III we consider the calculation of the electric field at the impurity due to the plasma ions, their screening, and their effective charge $\bar{Z}$. These are determined jointly by the physics of the plasma environment and by the basic atomic physics of the bare nuclear charge Z of the plasma ions. In Sec. IV we present numerical results of He, B, Be, and Li impurities in hydrogen plasmas and compare the effect of *ipp* corrections in the context of the Baranger-Mozer expansion taken to second order, and then in the WCS and APEX with all-order resummations. Section V contains a summary and conclusions.

II. FORMULATION OF THE MICROFIELD

The ion-microfield distribution $W(E)$ specifies the probability of occurrence of the static field E due to the field ions, at the site of the radiator. If $P(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_n)$ is the probability of the ionic configuration $(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_n)$, the microfield distribution is introduced by the definition

$$W(\mathbf{E})=\int d\mathbf{r}_1 d\mathbf{r}_2\cdots d\mathbf{r}_n P(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_n) \times\delta\left[\mathbf{E}-\sum_i \mathbf{E}_i\right]\ , \tag{2.1}$$

where $\mathbf{E}_i$ is the electric field at the impurity particle ("radiator") at the origin, arising from the ith perturber ion of the plasma, located at $\mathbf{r}_i$. Note that this *assumption of additivity* of the total field is a *weak electron-ion coupling assumption* which can still be used for strong coupling if a pseudopotential formulation is justifiable. For a homogeneous plasma $W(\mathbf{E})$ is spherically symmetric about the origin. The Fourier transform of $W(\mathbf{E})$ is given by

$$W(k)=W(\mathbf{k})=\int_0^\infty \exp\left[i\mathbf{k}\cdot\sum_i \mathbf{E}_i\right]P(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_n) \times d\mathbf{r}_1 d\mathbf{r}_2\cdots d\mathbf{r}_n\ ,$$

with

$$W(\mathbf{E})=W(E)=\frac{1}{2\pi^2}\int_0^\infty W(k)\frac{\sin(kE)}{kE}k^2 dk\ . \tag{2.2}$$

In the BM formalism the term $\exp(i\mathbf{k}\cdot\sum_i \mathbf{E}_i)$ is treated using the Ursell-Mayer cluster expansion. This leads to the result

$$W(k)=\exp[\tilde{S}(k)]=\exp\left[\sum_p \frac{(\bar{\rho})^p}{p!}w_p(k)\right]\ . \tag{2.3}$$

Here $\bar{\rho}$ is the mean ion density (we use $\bar{n}=\bar{Z}\,\bar{\rho}$ for the

mean free electron density, with $\bar{Z}$ the effective global ionic charge in the plasma. Details of the definition of $\bar{Z}$ will be discussed in Sec. III). The p-body microfield functions $w_p(k)$ are defined by

$$w_p(k)=\int \phi_1\phi_2\cdots\phi_p C_p(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_p)d\mathbf{r}_1 d\mathbf{r}_2\cdots d\mathbf{r}_p \ , \tag{2.4}$$

$$\phi_1=\phi(\mathbf{k},\mathbf{r}_1)=\exp(i\mathbf{k}\cdot\mathbf{E}_1)-1 \ ,$$

with the cluster functions

$$C_1(\mathbf{r}_1)=g(0,1) \ , \tag{2.5}$$

$$c_2(\mathbf{r}_1,\mathbf{r}_2)=g(0,1,2)-g(0,1)g(0,2) \ , \tag{2.6}$$

$$\begin{aligned} C_3(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=&g(0,1,2,3)-g(0,1,2)g(0,3)\\ &-g(0,1,3)g(0,2)-g(0,2,3)g(0,1)\\ &+2g(0,1)g(0,2)g(0,3) \ . \end{aligned} \tag{2.7}$$

Here $g(0,1)$ refers to the pair distribution function $g_{ip}(\mathbf{r}_0,\mathbf{r}_1)$ with the impurity ion at $\mathbf{r}_0$. Similarly $g(0,1,2)$ is a triplet distribution function $g_{ipp}(\mathbf{r}_0,\mathbf{r}_1,\mathbf{r}_2)$, while $g(0,1,2,3)$ denotes the four-particle function g_{ippp}. Note that we differ from the common notation of BM theory in retaining $g(1,2)$ for the PDF's, and similarly $h(1,2)$ for the total correlation function $g(1,2)-1$, as is customary in the theory of liquids.

In this approach no classical assumptions are made. The correct treatment of the electrons comes into the calculation of the ion distribution function $g(0,1)$, etc., and DFT theory is an appropriate method. Such calculations are necessary even in the lowest order [Eq. (2.5)] unless the impurity does not interact with the plasma (and hence does not undergo level broadening, etc.). However, in the usual case $g(0,1)$ is different from unity and a DFT-type calculation is needed even in the lowest approximation of the BM expansion. While the PDF's are easily available from DFT models of the plasma,[7] or from simulation data if the system were classical, the particle correlations of the form $g(0,1,2)$ which appear already in the second-order BM theory are not available, or, even if available, impractical to use. However, a simplified form of the BM series could be constructed by systematically using the Kirkwood approximation to reduce the higher-order correlation functions to those with two-particle correlation functions. It was shown in Ref. 6 how this simplified form of the BM series could be evaluated to all orders in what was called the weighted-chain-sum approximation. This simplified form of BM expansion is adequate for the low $\Gamma(<1)$ case treated here if the *ipp* corrections could be included. In the WCS approximation all the higher-order terms in the BM series, containing higher-order correlation functions, e.g., $h(1,2,3)$, are reduced to terms containing only pair correlation functions [e.g., $h(1,2,3)\rightarrow h(1,2)h(2,3)h(3,1)$]. The nth-order cluster function is then found to contain chainlike terms, viz., $h(1,2)h(2,3)h(3,4)\cdots h(n-1,n)$ +permutations, and other non-chainlike terms. We retain only the chainlike terms in each cluster function. The errors introduced via the Kirkwood-type approximation and the chain approximation are compensated by weighting the chain contribution so that the $(n+1)$th cluster function, when integrated over the $(n+1)$th particle coordinates, reduces correctly to the nth cluster function. Details of this weighted-chain-sum approximation are given in Ref. 5, where efficient numerical methods as well as comparison with Monte Carlo and APEX (Ref. 6) calculations are presented.

Let us consider the form of the second-order BM contribution and the supplementary term arising from the *ipp* correction. Using Eq. (1.2) to express the cluster function $C_2(\mathbf{r}_1,\mathbf{r}_2)$ we can write the second-order contribution $w_2(k)$ by

$$\begin{aligned} w_2(k)=\frac{1}{\Omega}\int &\phi(\mathbf{r}_1-\mathbf{r}_0)\phi(\mathbf{r}_2-\mathbf{r}_0)g_{ip}(0,1)g_{ip}(0,2)\\ &\times h_{pp}(1,2|r_0)d\mathbf{r}_0 d\mathbf{r}_1 d\mathbf{r}_2 \ , \end{aligned} \tag{2.8}$$

where

$$\phi(\mathbf{r}_1-\mathbf{r}_0)=\exp[i\mathbf{k}\cdot\mathbf{E}(1,0)]-1$$

and

$$h_{\rm pp}(1,2|\mathbf{r}_0)=g_{pp}(1,2|\mathbf{r}_0)-1 \ .$$

The electric field $\mathbf{E}(1,0)$ is the field at $\mathbf{r}_0$ due to the perturber ion at $\mathbf{r}_1$. Explicit expressions for this field will be given in Sec. III. The *ipp*-correction term now yields, in an abbreviated notation,

$$\begin{aligned} \delta w_2(k)=\frac{1}{\Omega}\int &\phi(0,1)\phi(0,2)g(0,1)g(0,2)\Delta h(1,2|\mathbf{r}_0)\\ &\times d\mathbf{r}_1 d\mathbf{r}_2 d\mathbf{r}_0 \ , \end{aligned} \tag{2.9}$$

where

$$\Delta h(1,2|\mathbf{r}_0)=h_{pp}(1,2|\mathbf{r}_0)-h^0_{pp}(|\mathbf{r}_1-\mathbf{r}_2|) \ .$$

A. Evaluation of particle correlations in the presence of the radiator

If we denote the impurity (radiator) by i located at $\mathbf{r}_0$, and the plasma particles (perturbers) by p, located at $\mathbf{r}_1$ and $\mathbf{r}_2$, then we with to evaluate

$$\Delta h_{pp}(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_0)=h_{pp}(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_0)-h^0_{pp}(|\mathbf{r}_1-\mathbf{r}_2|) \ .$$

Such an evaluation enables us to replace the usual Kirkwood form, Eq. (1.1), by the product form inclusive of *ipp* corrections, viz.,

$$g_{ipp}(0,1,2)=g_{ip}(0,1)g_{ip}(0,2)g_{pp}(1,2|\mathbf{r}_0) \ . \tag{2.10}$$

The study of this type of *ipp* corrections had recently become important in a different context, namely, in the study of the excitation spectrum of the correlated electron fluid associated with the fractional quantum Hall effect. The problem has been looked at using a two-component plasma model[10] and also using an inhomogeneous plasma model.[11] We also invoke these two approaches, clarify their relationship, and obtain results similar to those of Refs. 10 and 11, but differing in certain important aspects.

B. The two-component plasma model

Here we attempt to treat the impurity and plasma system as a two-component plasma made up of impurities (density ρ_i) and plasma ions of density ρ_p. The electrons do not appear, as their coordinates have been integrated out via the Kohn-Sham equations of DFT. The impurities and plasma ions interact via effective ion-ion potentials. The case where $\rho_i \to 0$ is the limit relevant to the problem of an impurity in a plasma.

Let the homogeneous plasma density $\bar{\rho}$ be explicitly denoted by ρ_p^0, with N particles in the volume Ω. The Ornstein-Zernike relation is

$$h_{pp}^0(\mathbf{r}_1,\mathbf{r}_2)=C_{pp}^0(\mathbf{r}_1,\mathbf{r}_2)+\rho_p^0\int C_{pp}^0(\mathbf{r}_1,r_3)h_{pp}^0(\mathbf{r}_3,\mathbf{r}_2)d\mathbf{r}_3\ , \tag{2.11}$$

where $h_{pp}^0(\mathbf{r}_1,\mathbf{r}_2)=h_{pp}^0(|\mathbf{r}_1-\mathbf{r}_2|)$, etc., since the plasma is homogeneous.

We remove one of the plasma particles and introduce an impurity ion. Then the new densities are

$$\rho_p=(N-1)/\Omega,\quad \rho_i=1/\Omega\ ,$$

therefore

$$\rho_p=\rho_p^0-\rho_i\ . \tag{2.12}$$

The new OZ relations are

$$h_{pp}(\mathbf{r}_1,\mathbf{r}_2)=C_{pp}(\mathbf{r}_1,\mathbf{r}_2)+\rho_p\int C_{pp}(\mathbf{r}_1,\mathbf{r}_3)h_{pp}(\mathbf{r}_3,\mathbf{r}_2)d\mathbf{r}_3 +\rho_i\int C_{pi}(\mathbf{r}_1,\mathbf{r}_3)h_{ip}(\mathbf{r}_3,\mathbf{r}_2)d\mathbf{r}_3\ , \tag{2.13}$$

$$h_{ip}(\mathbf{r}_1,\mathbf{r}_2)=C_{ip}(\mathbf{r}_1,\mathbf{r}_2)+\rho_p\int C_{ip}(\mathbf{r}_1,\mathbf{r}_3)h_{pp}(\mathbf{r}_3,\mathbf{r}_2)d\mathbf{r}_3\ . \tag{2.14}$$

The TCP is translationally invariant and here we have $h_{pp}(\mathbf{r}_1,\mathbf{r}_2)=h_{pp}(|\mathbf{r}_1,\mathbf{r}_2|)$, etc. There is no term in $C_{ii}(\mathbf{r}_1,\mathbf{r}_3)$ in the last equation since there are no impurity-impurity correlations in the limit of a single impurity in the integration volume Ω. Also, since $\rho_p=\rho_p^0-\rho_i$ we have

$$h_{pp}(\mathbf{r}_1,\mathbf{r}_2)=C_{pp}(\mathbf{r}_1,\mathbf{r}_2)+\rho_p^0\int C_{pp}(\mathbf{r}_1,\mathbf{r}_3)h_{pp}(\mathbf{r}_3,\mathbf{r}_2)d\mathbf{r}_3+\rho_i\int[C_{pi}(\mathbf{r}_1,\mathbf{r}_0)h_{ip}(\mathbf{r}_0,\mathbf{r}_2)-C_{pp}(\mathbf{r}_1,\mathbf{r}_0)h_{pp}(\mathbf{r}_0,\mathbf{r}_2)]d\mathbf{r}_0\ , \tag{2.15}$$

where we have used $\mathbf{r}_0$, instead of $\mathbf{r}_2$, in the last term involving the impurity density ρ_i.

If we write (2.15) as

$$h_{pp}(\mathbf{r}_1,\mathbf{r}_2)=h_{pp}^0(\mathbf{r}_1,\mathbf{r}_2)+\rho_p^i\Delta h_{pp}(\mathbf{r}_1,\mathbf{r}_2) \tag{2.16}$$

we see that $h_{pp}(\mathbf{r}_1,\mathbf{r}_2)\to h_{pp}^0(\mathbf{r}_1-\mathbf{r}_2)$ as $\rho_i\to 0$. The corrections (to leading order in ρ_i) to $h_{pp}^0(\mathbf{r}_1,\mathbf{r}_2)$ are hence contained in $\Delta h_{pp}(\mathbf{r}_1,\mathbf{r}_2)$ evaluated using zeroth-order quantities. Note that $\Delta h_{pp}(\mathbf{r}_1,\mathbf{r}_2)$ is an integral over the impurity position $\mathbf{r}_0$. However, the calculation of the correction to the microfield, $\delta W_2(E)$, requires $\Delta h_{pp}(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_0)$ prior to the $\mathbf{r}_0$ integration, as is clear from Eq. (2.9). Thus we identify $\Delta h(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_0)$ as

$$\Delta h(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_0)=\rho_i[C_{pi}(\mathbf{r}_1-\mathbf{r}_0)h_{ip}(\mathbf{r}_2-\mathbf{r}_0) -C_{pp}(\mathbf{r}_1-\mathbf{r}_0)h_{pp}(\mathbf{r}_2-\mathbf{r}_0)]\ . \tag{2.17}$$

Owing to the convolution structure of the OZ equation this expression needs to be symmetrized in $\mathbf{r}_1$ and $\mathbf{r}_2$. However, as far as the calculation of $\delta W_2(E)$ is concerned this is not required because $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_0$ are integrated over [see Eq. (2.9)].

We also note that if the impurity is replaced by a plasma particle the correction term $\Delta h(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_0)$ goes to zero as it should do.

In evaluating (2.17) to zeroth order, $C_{ip}(\mathbf{r}_1-\mathbf{r}_0)$ is available from Eq. (2.14) since $h_{ip}(\mathbf{r}_1-\mathbf{r}_0)$ is directly available from a DFT calculation for a plasma with the impurity at the origin. After some manipulation we get, in reciprocal space,

$$\Delta h(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_0)=\Delta h(\mathbf{r}_1-\mathbf{r}_0,\mathbf{r}_2-\mathbf{r}_0)\to\Delta h(\mathbf{q},\mathbf{q}')\ .$$

Retaining only terms in leading order in h, we get from (2.17).

$$\Delta h(q,q')=\rho_i[h_{ip}(q)h_{ip}(q')-h_{pp}(q)h_{pp}(q')]\ . \tag{2.18}$$

Hence we see that the leading correction is found to be second order in h_{ip}. Lauglin's result[10] is also found to be second order in h_{ip} but the correction term involving h_{pp}^2 is missing in his expressions.

C. The inhomogeneous plasma model

An alternative approach to the calculation of $h_{pp}(\mathbf{r}_1,\mathbf{r}_2)$ in the presence of an impurity is to treat the impurity and plasma system as an inhomogeneous plasma.[11] The impurity is treated as contributing an "external" potential which perturbs the homogeneous plasma. In Appendix A of Ref. 11 Fertig and Halperin (FH) develop the hypernetted-chain (HNC) equation and the OZ equation for an inhomogeneous system. These equations have also been discussed in Hansen and MacDonald.[13] If the external potential is $\phi(\mathbf{r})$, the inhomogeneous HNC and OZ equations are

$$g_{pp}^{\phi}(1,2)=\exp[-U(1,2)+h_{pp}^{\phi}(1,2)-C_{pp}^{\phi}(1,2)] \tag{2.19}$$

and

$$h_{pp}^{\phi}(1,2)=C_{pp}^{\phi}(1,2)+\int h_{pp}^{\phi}(1,3)\rho^{\phi}(3)C_{pp}^{\phi}(3,2)d\mathbf{r}_3\ , \tag{2.20}$$

respectively. In (2.19) $U(1,2)$ is the pair potential between two plasma ions in units of k_BT.

In Appendix D of FH, $h_{pp}^{\phi}(1,2)$ is evaluated as an expansion in terms of h_{ip} starting from the homogeneous

plasma value $h^0_{pp}(1,2)$. Instead of following Ref. 11 we proceed in a more direct manner.

The impurity (i.e., the external potential) is centered at the origin of coordinates. Suppressing the *pp* subscripts for brevity, we have, from Eq. (2.19),

$$\Delta h(1,2)=g^0(1,2)[\Delta h(1,2)-\Delta C(1,2)] =g^0(1,2)\Delta N(1,2) , \tag{2.21}$$

where $N(1,2)=h(1,2)-C(1,2)$ is the nodal function. Writing $\rho(r)=\bar{\rho}+\Delta\rho(r)$ we have, from Eq. (2.20),

$$\Delta h(1,2)=\Delta C(1,2)+\bar{\rho}\int \Delta C(1,3)h^0(3,2)d\mathbf{r}_3 +\bar{\rho}\int C^0(1,3)\Delta h(3,2)d\mathbf{r}_3 +\int C^0(1,3)\Delta\rho(3)h^0(3,2)d\mathbf{r}_3 . \tag{2.22}$$

Defining the double Fourier transform $f(\mathbf{q},\mathbf{q}')$ via

$$f(1,2)=(2\pi)^{-6}\int e^{-i\mathbf{q}\cdot\mathbf{r}_1}f(\mathbf{q},\mathbf{q}')e^{-i\mathbf{q}\cdot\mathbf{r}_2}d\mathbf{q}\,d\mathbf{q}' ,$$

Eq. (2.22) can be written as

$$\Delta h(\mathbf{q},\mathbf{q}')=S^0(\mathbf{q})\Delta C(\mathbf{q},\mathbf{q}')S^0(\mathbf{q}') +h^0(\mathbf{q})\Delta\rho(\mathbf{q}+\mathbf{q}')h^0(\mathbf{q}') . \tag{2.23}$$

This equation is identical with Eq. (D9) of Fertig and Halperin,[11] although different in appearance. The Fourier transform of Eq. (2.21) gives

$$\Delta h(\mathbf{q},\mathbf{q}')=\Delta N(\mathbf{q},\mathbf{q}') +(2\pi)^{-3}\int d\mathbf{Q}\,h^0(\mathbf{Q})\Delta N(\mathbf{q}-\mathbf{Q},\mathbf{q}+\mathbf{Q}) . \tag{2.24}$$

Using Eq. (2.23) we can write $\Delta C(\mathbf{q},\mathbf{q}')$ as

$$\Delta C(\mathbf{q},\mathbf{q}')=\Delta h(\mathbf{q},\mathbf{q}')S^0(\mathbf{q})S^0(\mathbf{q}') -C^0(\mathbf{q})\Delta\rho(\mathbf{q}+\mathbf{q}')C^0(\mathbf{q}') .$$

Therefore

$$\Delta N(\mathbf{q},\mathbf{q}')=[S^0(\mathbf{q})S^0(\mathbf{q}')-1]\Delta h(\mathbf{q},\mathbf{q}')S^0(\mathbf{q})S^0(\mathbf{q}') +C^0(\mathbf{q})\Delta\rho(\mathbf{q}+\mathbf{q}')C^0(\mathbf{q}') .$$

Using Eq. (2.24) we can finally write the change in the plasma-plasma correlations as

$$\Delta h(\mathbf{q},\mathbf{q}')=\Delta\rho(\mathbf{q}+\mathbf{q}')K(\mathbf{q},\mathbf{q}') , \tag{2.25}$$

where

$$K(\mathbf{q},\mathbf{q}')=h^0(\mathbf{q})h^0(\mathbf{q}')+S^0(\mathbf{q})S^0(\mathbf{q}')\int(2\pi)^{-3}d\mathbf{Q}\,C^0(\mathbf{q}-\mathbf{Q})h^0(\mathbf{Q})C^0(\mathbf{q}+\mathbf{Q}) +S^0(\mathbf{q})S^0(\mathbf{q})\int(2\pi)^{-3}d\mathbf{Q}\,h^0(\mathbf{Q})\left[\frac{S^0(\mathbf{q}-\mathbf{Q})S^0(\mathbf{q}+\mathbf{Q})-1}{S^0(\mathbf{q}-\mathbf{Q})S^0(\mathbf{q}+\mathbf{Q})}\right]K(\mathbf{q}-\mathbf{Q},\mathbf{q}+\mathbf{Q}) . \tag{2.26}$$

Using Eqs. (2.25) and (2.26) one can calculate $\Delta h(\mathbf{q},\mathbf{q}')$ as an expansion in powers of $h^0(q)$. Using Fertig and Halperin's form of $\rho(\mathbf{r})$ we have

$$\Delta\rho(\mathbf{r})=\bar{\rho}h_{ip}(\mathbf{r}) .$$

Hence, to leading order in (2.25),

$$\Delta h(\mathbf{q},\mathbf{q}')=h^0(\mathbf{q})h^0(\mathbf{q}')\Delta\rho(\mathbf{q}+\mathbf{q}') =O([\bar{\rho}(h^0)]^3) . \tag{2.27}$$

Thus the dependence to leading order obtained from the Fertig-Halperin treatment of the inhomogeneous plasma seems to be of the order of $[h(q)]^3$, while the TCP treatment (cf. previous discussion, or Laughlin's discussion in Ref. 9) lead to an $h^2(q)$ dependence.

The resolution of this inconsistency between the various results seems to lie in the exact definition of $\Delta\rho(\mathbf{r})$. In particular, the addition of an impurity atom, together with the removal of a plasma particle, leads to changes in the density of the order of $1/\Omega$, where Ω is the volume of integration. We believe that these $1/\Omega$ terms have not been handled in the same manner in Refs. 10 and 11. We note that the quantity $\Delta h(\mathbf{q},\mathbf{q}')$ calculated in the inhomogeneous plasma model is, in $\mathbf{r}$ space, $\Delta h(|\mathbf{r}_1-\mathbf{r}_0|,|\mathbf{r}_2-\mathbf{r}_0|)$ with $\mathbf{r}_0$ the origin of coordinates. Thus the $\Delta h(|\mathbf{r}_1-\mathbf{r}_2|)$ for the TCP model of Ref. 10 has to be recovered from that of Fertig and Halperin[11] by an integration over $\mathbf{r}_0$. Similarly, the modified density profile $\Delta\rho(|\mathbf{r}-\mathbf{r}_0|)$ when integrated over $\mathbf{r}_0$ and $\mathbf{r}$ should give the number of impurities in the volume Ω. This turns out to be zero in the Fertig-Halperin treatment, while it is of the order of unity in the Laughlin treatment and in ours. However, the reduction in plasma density from N/Ω to $(N-1)/\Omega$ is not included in Laughlin's treatment given in Ref. 10. Thus, while Refs. 10 and 11 are partially correct, they both miss certain terms which appear in the more complete expressions given here. Since $\Delta\rho(q+q')$ is needed in Eq. (2.25), in Sec. II D we review the density change due to the introduction of the impurity into the plasma.

D. Change in the density profile on impurity substitution

In order to understand the contributions to $\Delta\rho$ we consider two systems: (i) a system with $N+1$ plasma particles, $\rho_p^0=(N+1)/\Omega$, having no impurity but a plasma particle at the origin $\mathbf{r}_0$. (ii) A system with N plasma particles, $\rho_p=N/\Omega$, and with an impurity at r_0, i.e., $\rho_i=1/\Omega$. Thus we have, for the two systems, with $\rho^{(0)}(\mathbf{x})$, $\mathbf{x}=\mathbf{r}-\mathbf{r}_0$,

$$\rho^{(1)}=\rho_p^0[1+h^0_{pp}(\mathbf{x},\rho_p^0;N+1)] , \qquad \rho^{(2)}=\rho_p[1+h_{ip}(\mathbf{x},\rho_p;N)] . \tag{2.28}$$

The differences in the Ursell function of Eq. (2.6) for these two systems arise from (a) modifications in $g_{ip}(|\mathbf{r}_1-\mathbf{r}_0|)$ and $g_{ip}(|\mathbf{r}_2-\mathbf{r}_0|)$ which also involves an impurity correction, and (b) modification in $h_{pp}(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_0)$ when $\mathbf{r}_0$ contains the impurity. The DFT calculation explicit includes an impurity and hence item (a) does not arise in the present discussion. In the calculation of the difference

$$\Delta h(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_0)=h_{pp}(\mathbf{x}_1,\mathbf{x}_2,\rho^{(2)},N)-h_{pp}(\mathbf{x}_1,\mathbf{x}_2,\rho^{(1)},N+1)$$

the relevant density change can be written, on using the property $\rho_p=\rho_p^0-\rho_i$, as follows:

$$\begin{aligned}\Delta\rho&=\rho^{(2)}-\rho^{(1)}\\&=-\rho_i+\rho_p^0[h_{ip}(\mathbf{x},\rho_p^0,N+1)-h_{pp}(\mathbf{x},\rho_p^0,N+1)]\\&\quad+\rho_p^0O(h^2)+\rho_iO(h)\ .\end{aligned}\tag{2.29}$$

The first term is due to the replacement of a plamsa particle with an impurity atom in a homogeneous system. The second term describes the rearrangement of the particle density around the particle at the origin. It corresponds to a purely *inhomogeneous* effect in a system with a *constant* number of particles. As we are interested only in the limit $\rho_i\to 0$, only the linear response to $\Delta\rho$ is relevant. Hence, writing (2.29) as

$$\Delta\rho=-\rho_i+\Delta\rho^{\mathrm{IHP}}$$

we can treat the effect of ρ_i and $\Delta\rho^{\mathrm{IHP}}$ separately. That is, we use the TCP to evaluate the effect of ρ_i and the inhomogeneous plasma model to evaluate the effect of $\Delta\rho^{\mathrm{IHP}}$. Note that we could have in principle evaluated the effect of $\Delta\rho^{\mathrm{IHP}}$ *using only the TCP equations* if an iterative calculation involving Eqs. (2.13) and (2.14) were to be carried out. But the present procedure is easier and enables us to retain an expansion defined to a specific order in perturbation theory.

E. Final expressions for $\Delta h(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_0)$

In view of the preceding discussion, the *ipp*-correction term to be evaluated can be written as

$$\Delta h_{pp}(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_0)=\Delta h_{pp}^a+\Delta h_{pp}^b\ ,\tag{2.30}$$

where

$$\begin{aligned}\Delta h_{pp}^a(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_0)&=h_{ip}(|\mathbf{x}_1|)h_{ip}(|\mathbf{x}_2|)\\&\quad-h_{pp}^0(|\mathbf{x}_1|)h_{pp}^0(|\mathbf{x}_2|)\end{aligned}\tag{2.31}$$

and

$$\begin{aligned}&\Delta h_{pp}^b(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_0)\\&\quad=\int\{h_{pp}^0(|\mathbf{x}_1-\mathbf{x}_3|)\\&\qquad\times[h_{ip}(|\mathbf{x}_3|)-h_{pp}(|\mathbf{x}_3|)]h_{pp}^0(|\mathbf{x}_3-\mathbf{x}_2|)\}d\mathbf{x}_3\ ,\end{aligned}\tag{2.32}$$

with

$$\mathbf{x}_1=\mathbf{r}_1-\mathbf{r}_0\ ,$$

etc.

Numerical calculation of the contribution to the microfield arising from (2.32) involves the expansion of $\Delta\rho^{\mathrm{IHP}}(\mathbf{q}-\mathbf{q}')$ in Legendre polynomials up to and including order 3. The calculations show that the *ipp* correction arising from the inhomogeneous term is quite small, and hence the restriction of these calculations to lowest order is well justified. Other small corrections (e.g., changes to the pair potential) which appear in this context have also been neglected.

III. CALCULATION OF THE ELECTRIC FIELDS

The microfield calculation requires the value of the electric field **E** due to the perturbing ions acting on the impurity ion at the origin. If the electron-ion coupling is weak we may write

$$\mathbf{E}=\sum_p(Z^*/\mathbf{r}_p)\exp(-\lambda r_p)\ ,\tag{3.1}$$

where the summation is over all the perturber positions $\mathbf{r}_p$. In (3.1) λ is a screening constant and Z^* is a mean ionic charge. In the weak-coupling limit there is no serious ambiguity regarding Z^* or λ. The mean ionic charge is calculated via a Saha-like equation and λ is obtained from linear screening theory. In such a theory Z^* becomes essentially identical to the global value $\bar{Z}$ such that the free-electron density $\bar{n}=\bar{Z}\,\bar{\rho}$, with $\bar{\rho}$ the perturber-ion density far away from the impurity. In a dense plasma this simple picture is no longer valid. Bound states of a given perturber ion may extend[14] beyond a nearest-neighbor distance and the concept of ions with a compact shell of bound states may not be valid. The screening of a given ion due to the free electrons will be nonlinear and also strongly dependent on the configuration of the other ions around it (uniform background models are invalid). Hence electron screening cannot be specified without reference to the ionic correlation functions of the system. A naive approach to such a coupled system will not yield the additive structure of the electric fields assumed in Eq. (3.1).

Our approach to such systems is essentially to construct the structure of the perturber ions, i.e., their bound- and free-state densities, correlation functions, etc., out of the total electron and ion densities $n(r)$, $\rho(r)$ which are considered to be made up of superpositions of individual charge densities. Hence a superposition principle holds, essentially as in second-order pseudopotential theory, although we do not need to assume the validity or the existence of such pseudopotentials. We remind the reader that the plasmas that we are studying here have ion-ion coupling $\Gamma<1$ and hence the deconvolution approach used here could be considered an excellent procedure.

A DFT calculation for a plasma treats the whole plasma contained in a "correlation sphere" of radius R and volume Ω about a nucleus of charge Z placed at the origin. The correlation sphere radius R is such that $g(R)$ is essentially unity, i.e., Ω is big enough to include characteristic lengths associated with ionic and electronic correlations. Typically R is some 5 to 10 Wigner-Seitz radii and would involve a large number of atoms and electrons.

The single-particle (electron) spectrum and ion-correlation functions associated with the central ion are obtained from the DFT calculation. The calculation yields a free-electron (energy $\epsilon>0$) density $n^f(r)$ and a bound electron ($\epsilon<0$) density $n^b(r)$. These densities are for the total system and need to be decomposed into contributions from individual ions. Since, in the homogeneous plasma all ions (including the central ion) are equivalent, the total densities can be considered as obtained from a linear superposition of individual spherical densities. Thus, if $\bar{n}$ is the mean density and $\Delta n^f(r)=n^f(r)-\bar{n}$, we have

$$\Delta n^f(r)=\Delta n_p^f(r)+\sum_p{}' \Delta n_p^f(|\mathbf{r}-\mathbf{r}'|) , \tag{3.2}$$

where the primed p summation is over all the plasma ions at position $\mathbf{r}_p$, excluding the origin. Thus $\Delta n_p^f(|r-r_p|)$ is the free-electron density pileup (displaced density) around an individual ion at the location $\mathbf{r}_p$ *in the plasma.* Note that this $\Delta n_p(\mathbf{r})$ has to be calculated for each environment, with all the other charges in place, and hence need not be the same as, say, the displaced electron density $\Delta n_f^f(r)$ around an isolated ion placed in a uniform responding *jellium* background with the same density $\bar{n}$ and temperature T.

The summation over ion positions in Eq. (3.2) can be written in terms of the ion-distribution function. Hence Fourier transformation of (3.2) gives

$$\Delta n_p^f(q)=\Delta n^f(q)/[1+\bar{\rho}h(q)] . \tag{3.3}$$

This displaced electron density depends explicitly on the ion correlation function $h(q)$ and implicitly on the total plasma environment since $\Delta n^f(q)$ is an electron density calculated from the self-consistent solution of the Schrödinger equation for the electrons and ions inside the correlation sphere. We refer to the calculation of $\Delta n_p^f(q)$ given above as the *deconvoluted plasma model* of the displaced density.

Since the total bound electron density $n^b(r)$ is known, an effective ionic charge

$$\bar{Z}=Z-n_p^b , \tag{3.4}$$

where n_p^b is the *number* of bound electrons associated with a single ion, can be defined. Since the total bound density distribution $n^b(r)$ is known, the *number* n_p^b of bound electrons contained within a radius r^b is

$$n_p^b=\int_0^{r^b} 4\pi r^2 n^b(r)dr \tag{3.5}$$

and satisfies the neutrality condition

$$Z=n_f+n_p^b , \tag{3.6}$$

where n_f is the number of free electrons in the sphere of radius r^b. Thus

$$n_f=(r^b/r_s)^3, \quad r_s^3=3/(4\pi\bar{n}) . \tag{3.7}$$

r^b may be thought of as the size (radius) of the perturber ion, carrying a cloud of n_p^b *bound* electrons. In the present case r^b is simply the Wigner-Seitz radius

$$r_{\mathrm{WS}}=[3/(r\pi\bar{\rho})]^{1/3} . \tag{3.8}$$

Now that the bound- and free-electron distributions associated with a perturber ion in a strongly coupled plasma have been defined, we can define the electric field $E_p(\mathbf{r})$ at the origin, due to a single perturber ion at a distance $\mathbf{r}$ from the origin, as being

$$E_p(r)=-\frac{\bar{Z}}{r^2}+\frac{1}{r^2}\int_0^r \Delta n_p^f(x)4\pi x^2 dx$$
$$=-\frac{\bar{Z}}{r^2}q(r) \tag{3.9}$$

for $r>r^b$. For perturbers approaching the central ion so that $r<r^b$, i.e., for penetration of the bound electron shell, this equation is not suitable. In any case, the probability of such close approaches is very small since $g_{ip}(r)$ rapidly drops to zero for $r<r_{\mathrm{WS}}$. Further, for such close approaches, the microfield calculated at the origin will not be a good approximation to the microfield "felt" by an electron in, say, a $2p$-bound state whose Stark shift is to be calculated. Then we need concepts which go beyond the microfield model and we shall not consider this case in this paper.

Returning to the second-order BM expression and the *ipp* correction given by Eqs. (2.8) and (2.9), the electric fields $E(1,0)$ [i.e., $E(\mathbf{r}_1)$], etc., are now identified with the physical fields given by Eq. (3.9). Hence the microfield is completely and unambiguously defined.

IV. NUMERICAL RESULTS FOR THE MICROFIELD

In this section we present the microfields in a hydrogen plasma at a density such that $r_s=1$ a.u., i.e., the mean electron density $\bar{n}=1.611\times10^{24}$ electrons/cm^3, and the temperature T such that $\beta^{-1}=50$ eV. This corresponds to $T/T_F=1$ where T_F is the Fermi temperature, i.e., $k_B T_F=E_F$ is the Fermi energy. Under these conditions the H plasma is fully ionized and $\bar{Z}=1$. The use of a fully ionized plasma makes the plasma model closer to what is possible in traditional microfield calculations. The high electron density ($r_s=1$) would suggest that linear screening theory may not be too bad and hence these calculations can in principle be compared with traditional microfield calculations where linear screening assumptions are made. Note that the unscreened ion-ion coupling parameter is $\Gamma=0.544$ and hence ion correlations begin to be important.

The microfields are calculated at the impurities He, Li, Be, and B, and also at a proton (H^+) although, of course, such a radiator could only support free-free processes. In dealing with such impurity ions we could either assume that these ions are "given" in specific electronic configuration, *or* we could assume that they are taken in their "average atom" configurations. The use of an average atom configuration implies that there are many impurities in the system, even though ρ_i is small, and hence the possible impurity configurations average over. Hence the impurity-plasma pair distribution functions $g_{ip}(r)$ are calculated using a density-functional description of the impurity electronic structure, with the impurity energy

TABLE I. Details of the impurities introduced into a fully ionized hydrogen plasma such that $r_s=1$, i.e., $\bar{n}_e=1.6\times10^{24}$ electrons/cm^3; $T/T_F=1$, i.e., $\beta^{-1}=50$ eV; and $\Gamma=0.544$. The total *number* of electrons bound by the impurity ion and the displaced ion density $\bar{\rho}g_{ii}(r)$ is N_B. Also, $\Delta\rho(q=0)$ is the additional number of plasma ions displaced from the correlation sphere on introducing the impurity. Thus $\Delta\rho=\bar{\rho}\int[g_{ip}(r)-g_{pp}(r)]r^2dr$. The bound state ($1s$) energy is given in atomic units (27.21 eV).

	H	He	Li	Be	B
ε_{1s} (a.u.)		−0.2098	−1.1790	−2.8024	−5.1800
N_B	0	1.0484	1.3024	1.6375	1.8855
$\Delta\rho(q=0)$	0	−0.3488	−0.6132	−0.8420	−1.0865

levels occupied by mean electron numbers (rather than by integer or zero occupations). The impurities He, Li, Be, and B support a $1s$ bound state, but the host plasma is fully ionized (see Table I for details). Although these impurities would not give line spectra, they are used here purely for illustration of how the microfields would be affected by the *ipp* correction.

We shall first discuss the calculation of the electric fields that go into the construction of the microfields. Then we examine the second-order Baranger-Mozer microfield [i.e., sum of $\bar{\rho}w_1+(\bar{\rho}^2/2)w_2$] with and without the *ipp* corrections. We shall also estimate the contributions due to higher-order terms (beyond second order) in the BM expansion using the WCS approximation and two versions of the APEX model.

A. Results for the electric fields

The electric field at the impurity due to a single perturber ion of charge $\bar{Z}$ at r is given by Eq. (3.9), i.e.,

$$E(r)=-\frac{\bar{Z}}{r^2}\left[1-\frac{1}{\bar{Z}}\int_0^r\Delta n^f(x)4\pi x^2dx\right]$$
$$=-\bar{Z}q(r)/r^2\,, \tag{4.1}$$

where $\Delta n^f(x)$ is the screening charge associated with a perturber ion. Thus $\Delta n^f(x)$ is $\Delta n_j(x)$ or $\Delta n_p(x)$ for the jellium model or for the plasma model, respectively (we drop the superscript f for simplicity). The displaced electron density $\Delta n_p(r)$ derived from the plasma according to Eq. (3.3) is shown in Fig. 1, while the difference $\Delta n_j(r)-\Delta n_p(r)$, weighted with r^2 is shown in Fig. 2. It is clear that for the hydrogen plasma studied here ($\Gamma=0.544$, $r_s=1$, $T/T_F=1$, $\bar{Z}=1$) the jellium model provides a good approximation to the deconvoluted plasma model. The screening function $q(r)$ calculated from the plasma model is shown in Fig. 3. Differences between the jellium and plasma models become more apparent in the electric fields (Table II) and in the calculated microfields (to be discussed in Sec. IV B). If the calculation had been carried out for a hydrogen plasma, which is slightly less dense, or more hot, the jellium results would be

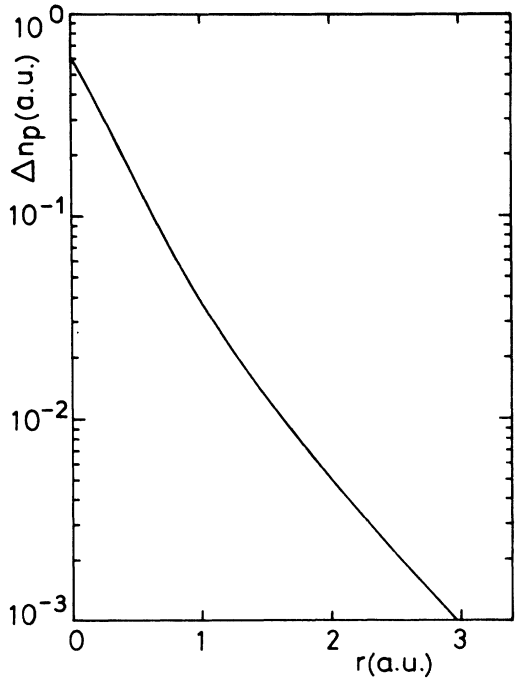

FIG. 1. Displaced electron density Δn_p attributed to a plasma hydrogen ion, obtained by deconvolution of the electron density displacement given by the DFT calculation for the hydrogen plasma ($r_s=1$, $T/T_F=1$, $\bar{Z}=1$, $\Gamma=0.544$).

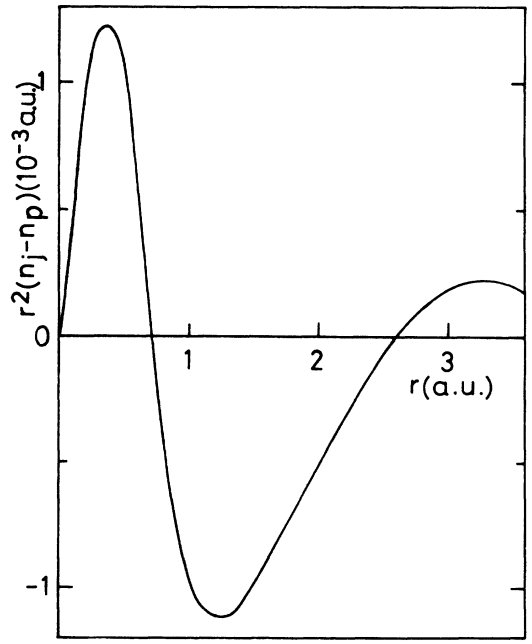

FIG. 2. Differences between the densities Δn_j (jellium background) and Δn_p (from the deconvoluted DFT calculation for the plasma).

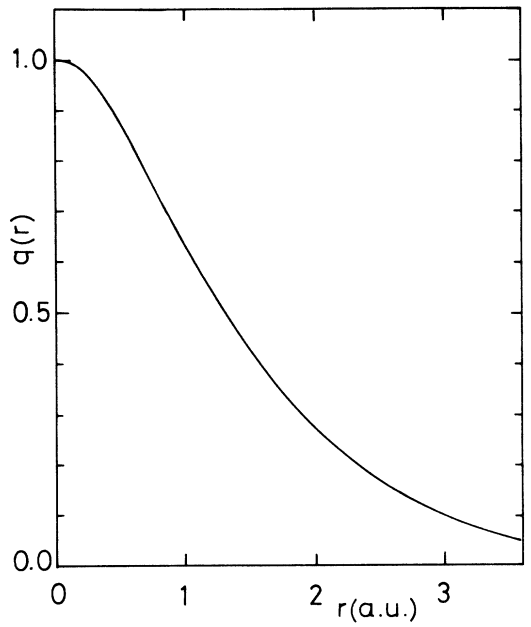

FIG. 3. Electric field screening function, Eq. (4.1), $q(r)=r^2E/\bar{Z}$ for the H ion (deconvoluted plasma model).

significantly different from those of the deconvoluted plasma results. This is because although the H^+ ions in the plasma do not support any bound states, an H^+ ion in jellium already begins to support an extremely shallow bound state ($\epsilon_{1s}=-0.000\,66$ hartrees, ~ 0.03 eV) even at the chosen conditions of $r_s=1$ and $T/T_F=1$. For larger values of r_s and T, a definite bound state will arise in the jellium case, before such a bound state arises in the plasma case.

B. Second-order BM microfield and the *ipp* correction

As is customary, we report the microfield probabilities $W(E/E_0)$, where E_0 is the standard Holzmark field given by

TABLE II. Comparison of displaced electron densities and screened electric fields at distances r (a.u.) from a hydrogen ion (perturber) calculated from the uniform-jellium-background model and from the deconvoluted plasma model. The electric field is given by $q(r)=-r^2E(r)/\bar{Z}$, Eq. (4.1).

r	Jellium		Plasma	
(a.u.)	$\Delta n_j(r)$	$q_j(r)$	$\Delta n_p(r)$	$q_p(r)$
0.003	0.6921	1.0000	0.6177	1.0000
0.102	0.5260	0.9975	0.4888	0.9977
0.205	0.3882	0.9833	0.3640	0.9847
0.304	0.2860	0.9560	0.2709	0.9593
0.510	0.1484	0.8677	0.1444	0.8756
1.025	0.0337	0.6127	0.0346	0.6230
1.522	0.0117	0.4143	0.0122	0.4205
2.000	0.0049	0.2716	0.0050	0.2751
2.539	0.0020	0.1607	0.0020	0.1639
3.018	0.0009	0.0957	0.0009	0.1003

$$E_0=Z/r_0^2,\quad r_0=0.999\,117\,8r_s\ , \tag{4.2}$$

writing $\tilde{E}=E/E_0$, $x=kE_0$, we have, from Eqs. (2.2) and (2.3),

$$W(\tilde{E})=\frac{2}{\pi}\tilde{E}\int_0^\infty dx\, x\sin(\tilde{E}x)W(x)\ . \tag{4.3}$$

The BM microfield calculated up to second order is then given by

$$W(x)=W_2(x)=\exp\left[\bar{\rho}w_1(x)+\frac{\bar{\rho}^2}{2}w_2(x)\right]\ . \tag{4.4}$$

Using (4.4) in (4.3) we get $W_2(\tilde{E})$. Although the impurities (see Table I) are denoted by H, He, Li, Be, and B, they have mean charges $\bar{Z}_i$ ranging from 1 for hydrogen to $\bar{Z}\simeq 3.2$ for boron. The case of the "H-impurity" really corresponds to a homogeneous plasma. The impurity electronic configuration enters into the microfield essentially through the determination of $g_{ip}(r)$. These PDF's are shown in Fig. 4. The left-most curve is $g_{\rm HH}(r)$, i.e., the PDF of the homogeneous fully ionized hydrogen plasma $g^0_{pp}(r)$. The right-most curve is for the Boron impurity, i.e., $g_{\rm BH}(r)$.

Table III presents the results for $W_2(\tilde{E})$ for the radiators (H, He, Li, Be, B) under study. In each case, column 1 gives $W_2(\tilde{E})$ calculated using the jellium model electric field. This is shown graphically in Fig. 5. Column 2 of Table III gives $W_2(\tilde{E})$ calculated with the deconvoluted plasma model of the electric field. The differences between these two models are more significant for boron than for the H "radiator" (this is just a proton—it can only support free-free processes). But even for the hydrogen case (homogeneous plasma), the differences are about 4% at $\tilde{E}=0.16$. Hence it is clear that the accuracy of the jellium model (uniform background) is questionable for

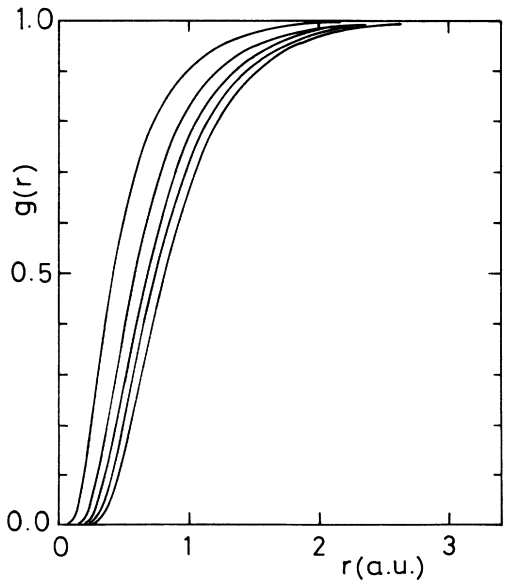

FIG. 4. Distribution function $g_{ip}(r)$ for various impurities i=H,He,Li,Be,B are given from left to right. The plasma particles p are H^+ ions ($r_s=1$, $T/T_F=1$).

TABLE III. The second-order BM microfield probability distribution at H, He, Li, Be, and B impurities in a hydrogen plasma ($r_s=1$, $T/T_F=1$, $\bar{Z}=1$). Column 1 is evaluated using the jellium electric field (see Table II). Column 2 is evaluated using the deconvoluted plasma electric field. Column 3 is obtained by adding the *ipp* correction to column 2. This is zero for the homogeneous plasma (i.e., H impurity). E_0 is the reference field Ze^2/r_0^2. The maximum probability W_m occurs at the field E_m.

	H			He			Li			Be			B		
E/E_0	1	2	3	1	2	3	1	2	3	1	2	3	1	2	3
0.0314	0.0185	0.0177		0.0235	0.0225	0.0234	0.0279	0.0267	0.0287	0.0322	0.0308	0.0339	0.0372	0.0356	0.0405
0.1571	0.3507	0.3377		0.4388	0.4229	0.4369	0.5136	0.4952	0.5246	0.5830	0.5623	0.6084	0.6637	0.6406	0.7073
0.3142	0.7539	0.7344		0.9073	0.8851	0.9041	1.0255	1.0015	1.0352	1.1265	1.1014	1.1464	1.2357	1.2097	1.2639
0.6283	0.7631	0.7580		0.8326	0.8297	0.8284	0.8680	0.8667	0.8582	0.8875	0.8879	0.8702	0.8989	0.9015	0.8714
0.9425	0.5086	0.5128		0.5097	0.5154	0.5085	0.4969	0.5047	0.4908	0.4790	0.4878	0.4682	0.4551	0.4646	0.4399
1.2566	0.3254	0.3299		0.3032	0.3090	0.3034	0.2804	0.2865	0.2777	0.2588	0.2652	0.2546	0.2341	0.2404	0.2297
1.8850	0.1413	0.1444		0.1161	0.1195	0.1175	0.0979	0.1000	0.0978	0.0819	0.0840	0.0823	0.0662	0.0681	0.0672
E_m/E_0	0.4515	0.4581		0.4205	0.4263	0.4273	0.3995	0.4050	0.4063	0.3828	0.3876	0.3892	0.3656	0.3707	0.3727
W_m	0.8482	0.8339		0.9836	0.9666	0.9652	1.0850	1.0664	1.0640	1.1715	1.1516	1.1484	1.2652	1.2440	1.2400

these systems, although the differences between Δn_j and Δn_p seem to be small.

In column 3 of Table III we give the total Baranger-Mozer microfield up to second order and including the *ipp* correction. The principal correction to the PDF which produces this *ipp* correction is $\Delta h(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_0)$, calculated using the TCP model. We show in Fig. 6 the form of this correlation correction in the case of the boron impurity, for several simple configurations. In Table III, we see that in the case of He and Li the deconvolution effects and *ipp* corrections seem to go in opposite directions and hence the simple uncorrected jellium calculation (column 1) seems to agree with the calculation in column 3. However, this is seen not to be the case in Be and B, where the *ipp* correction dominates the deconvolution effects. In fact, for higher-Z ions the *ipp* correction would be expected to be even more important. The full *ipp* correction was defined in Eqs. (2.29) and (2.9), and is the sum of a correction $\delta W_2(\tilde{E})$ calculated via the TCP model and another smaller contribution $\delta W_2(\tilde{E})$ using the IHP model. Table IV presents these two contributions separately. From these two tables it is clear that the *ipp* correction becomes increasingly important along the sequence He to B, as the field of maximum probability moves to lower values. In the case of the plasma with the boron impurity the largest correction to $W(E)$ is of the order of 10%. Thus the *ipp* corrections need to be taken into account.

C. All-order corrections to the second-order BM microfields

Having obtained the BM microfield up to second order inclusive of *ipp* corrections, it is of interest to determine the magnitude of the corrections arising from a resummation of the remainder, i.e., $\Delta W_\infty = W_\infty - W_2$. The value of ΔW_∞ will clearly depend on the method of resummation used. We will examine ΔW_∞ calculated from the weighted-chain-sum approximation and two forms of the adjustable parameter exponential approximation.[6]

The all-order microfield probability function $W_\infty(E)$ is calculated from the sum $\tilde{S}(k)$ of Eq. (2.3), viz.,

$$\tilde{S}(k)=\sum_n \tilde{S}_n(k)=\sum_n \frac{\bar{\rho}^n}{n!} w_n(k) \ . \tag{4.5}$$

The n-body microfield function $w_n(k)$, given by Eq. (2.4), involves the Ursell function $C_n(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_n)$. The WCS approximation is discussed in detail in Ref. 5. It proceeds by approximating the nth Ursell function by a sum of chainlike contribution arising from the $n-1$ bonds in the cluster,

TABLE IV. The change in the second-order BM microfield distribution $\Delta W_2(E)$ due to the *ipp* correction. Column (1) contains the TCP correction arising from $h_{ip}(1,0)h_{ip}(2,0)-h^0_{pp}(1,0)h^0_{pp}(2,0)$. Column (2) contains the IHP contribution arising from $\int d\mathbf{r}_3 h_{pp}(1,3)[h_{ip}(3,0)-h_{pp}(3,0)]h_{pp}(3,2)$. See Eqs. (2.29)–(2.31).

	He		Li		Be		B	
E/E_0	(1)	(2)	(1)	(2)	(1)	(2)	(1)	(2)
0.0314	0.0010	−0.0001	0.0022	−0.0002	0.0035	−0.0004	0.0054	−0.0005
0.1571	0.0162	−0.0022	0.0332	−0.0038	0.0514	−0.0053	0.0737	−0.0070
0.3142	0.0214	−0.0024	0.0377	−0.0040	0.0501	−0.0051	0.0603	−0.0061
0.6283	−0.0015	0.0002	−0.0092	0.0007	−0.0191	0.0014	−0.0323	0.0022
0.9425	−0.0078	0.0009	−0.0154	0.0015	−0.0216	0.0020	−0.0271	0.0024
1.2566	−0.0062	0.0006	−0.0098	0.0010	−0.0117	0.0011	−0.0121	0.0014
1.8850	−0.0022	0.0002	−0.0025	0.0003	−0.0020	0.0003	−0.0011	0.0002
2.5133	−0.0006	0.0000	−0.0002	0.0000	0.0002	0.0001	0.0009	0.0000

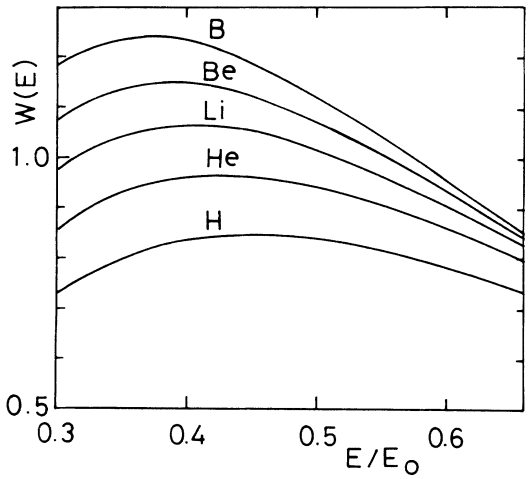

FIG. 5. BM-microfield distribution $W_2(E)$ without the *ipp* correction, near the maximum, for H, He, Li, Be, and B impurities in the hydrogen plasma ($r_s=1$, $T/T_F=1$). The electric field is from the jellium model (see column 1 of Table III).

$$C_n(\mathbf{r}_1,\mathbf{r}_2,\ldots,r_n)=U_n[h(1,2)h(2,3)\cdots h(n-1,n)] + \text{permutations} . \quad (4.6)$$

The weight factor U_n attached to the decomposition of the nth Ursell term is chosen to satisfy the sequential relation between Ursell functions given by

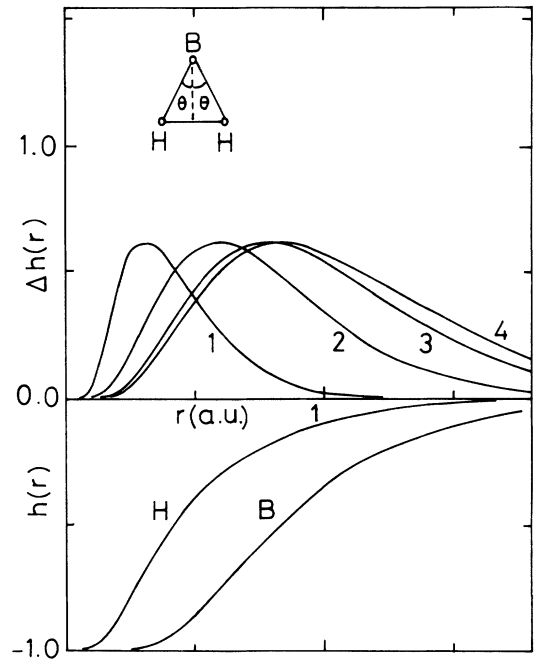

FIG. 6. The dominant *ipp* correction, Eq. (2.30), $\Delta h^a_{pp}(\mathbf{r}_1,\mathbf{r}_2|\mathbf{r}_0)$ obtained from the TCP model shown (upper panel) as a function of $r=|\mathbf{r}_1-\mathbf{r}_2|$ for the isosceles configuration (inset) with a boron ion at $\mathbf{r}_0$ and two protons at $\mathbf{r}_1$ and $\mathbf{r}_2$. The curves 1,2,3,4 correspond to $\theta=\pi/8$, $\pi/4$, $3\pi/8$, and $\pi/2$, respectively. In the lower panel the total correlation function $h^0_{pp}(r)$ and $h_{ip}(r)$, where $p=\mathrm{H}^+$ and $i=$boron, are displayed as a function of r.

TABLE V. All-order resummation beyond second order of the BM microfield distribution at H→B impurities in a hydrogen plasma. That is, $\Delta W_\infty = W_\infty(E)-W_2(E)$, without *ipp* corrections, is evaluated using two forms of APEX (Ref. 7) and WCS (Ref. 5). In APEX1, electron screening is approximated by constant $\lambda=\lambda^e_D$, where λ^e_D is the Debye screening length. In APEX2, $\lambda=1.5\lambda^e_D$. The APEX parameter α [see Eq. (4.12)] is then evaluated as discussed in Sec. IV. See also Fig. 7.

	Hydrogen			Helium			Lithium			Beryllium			Boron		
E/E_0	APEX1	APEX2	WCS	APEX1	APEX2	WCS	APEX1	APEX2	WCS	APEX1	APEX2	WCS	APEX1	APEX2	WCS
0.0314	0.0047	0.0043	0.0005	0.0054	0.0049	0.0007	0.0058	0.0054	0.0009	0.0061	0.0056	0.0011	0.0064	0.0059	0.0013
0.1571	0.0622	0.0565	0.0080	0.0640	0.0583	0.0109	0.0639	0.0580	0.0132	0.0628	0.0568	0.0151	0.0608	0.0547	0.0170
0.3142	0.0533	0.0474	0.0096	0.0395	0.0343	0.0117	0.0279	0.0233	0.0188	0.0179	0.0138	0.0114	0.0074	0.0037	0.0107
0.6283	−0.0178	−0.0171	−0.0015	−0.0255	−0.0242	−0.0036	−0.0268	−0.0268	−0.0055	−0.0261	−0.0240	−0.0069	−0.0236	−0.0212	−0.0083
0.9425	−0.0231	−0.0212	−0.0045	−0.0201	−0.0181	−0.0050	−0.0167	−0.0147	−0.0053	−0.0126	−0.0107	−0.0052	−0.0085	−0.0067	−0.0049
1.2566	−0.0154	−0.0139	−0.0034	−0.0109	−0.0096	−0.0027	−0.0076	−0.0065	−0.0024	−0.0060	−0.0050	−0.0020	−0.0044	−0.0036	−0.0014
1.8850	−0.0028	−0.0021	−0.0013	0.0003	0.0009	−0.0005	0.0025	0.0027	0.0	−0.0041	−0.0042	−0.0002	0.0052	0.0053	0.0003

$$\bar{\rho}\int U_{n+1}(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_{n+1})d\mathbf{r}_{n+1} = -nU_n(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_n)\ . \quad (4.7)$$

The decomposition (4.6) involves a Kirkwood-like decomposition of higher-order correlation functions to yield a result in terms of the pair correlation functions $h(12)$. It was found that the imposition of the sequential relation by choosing the weight factor (4.6) helps to overcome some of the shortcomings of the Kirkwood-like decomposition and the restriction of the sum to chainlike graphs. In principle, the $h(12)$ terms in the WCS approximation also need to be modified by *ipp* corrections. In practice, we calculate $W_\infty^{\rm WCS}(E)$ using the usual WCS approximation and $W_2^{\rm BM}(E)$ using the usual simplified BM calculation, and obtain $\Delta W_\infty^{\rm WCS}(E)$ from $W_\infty^{\rm WCS}(E) - W_2^{\rm BM}(E)$. That is, *ipp* corrections are *ignored* in the terms beyond second order in the all-order evaluation of the microfield probability function. If W_2 and W_∞ are known, and if the *ipp* correction in second order is δW_2, a proportionate *ipp* correction for the terms beyond W_2 would be estimated as $\delta W_2(\Delta W_\infty/W_2)$. The maximum value of δW_2 found in Table III is about 10% and hence the estimated *ipp* correction on the terms beyond second order is less than 0.3%. Thus we did not attempt to systematically include the *ipp* correction into the WCS calculation. Calculated values of $\Delta W^{\rm WCS}$ are given in column 3 of Table V.

In the APEX method the actual single-particle electric field $E(r)$, given by Eq. (4.1), is replaced by an effective field E^*. The all-order sum $\tilde{S}(k)$ of Eq. (4.5) is given by the formula

$$\tilde{S}(k)=4\pi\bar{\rho}\int_0^\infty r^2dr\, g_{ip}(r)\frac{E(r)}{E^*(r)}[J_0(kE^*)-1]\ . \quad (4.8)$$

We define [c.f. Eq. (4.1)]

$$\epsilon=-q(r)/r^2,\ \text{i.e.,}\ E=\bar{Z}\epsilon \qquad x=k\bar{Z}/r_0^2,\ \text{i.e.,}\ x=kE_0\ , \quad (4.9)$$

then the argument $kE=xr_0^2\epsilon$. The effective field E^* is determined so as to give the correct coefficient of the term in x^2 in the expansion of $\tilde{S}(k)$ for $k\to 0$. In the classical one-component plasma (OCP) this coefficient T_2 is known exactly via the second-moment sum rule. For the electron-ion plasma considered here, a less exact procedure is followed. We can calculate $T_2^{\rm APEX}$ in this case from the first two terms of the BM series, since only $\tilde{S}_1$ and $\tilde{S}_2$ contribute to second order in x. These contributions can be recast into the form

$$x^2T_2^{\rm BM}=-x^2r_0^2\tfrac{2}{3}\bar{\rho}\left[\pi\int_0^\infty g_{ip}(r)\frac{q^2(r)}{r^2}dr-2\bar{\rho}\int_0^\infty q^2dqh^0(q)\left[\int_0^\infty g_{ip}(r)q(r)j_1(qr)dr\right]^2\right], \quad (4.10)$$

where $h^0(q)$ is $h_{pp}^0(q)$ and arises from the Krirkwood decomposition of the $g_{ipp}(\mathbf{r}_0,\mathbf{r}_1,\mathbf{r}_2)$ term in the second-oder Ursell function (that is, no *ipp* correction is introduced). The contribution to x^2 in APEX is given by

$$x^2T_2^{\rm APEX}=-x^2r_0^2\tfrac{2}{3}\bar{\rho}\pi\int_0^\infty g_{ip}(r)\epsilon^*(r)\epsilon(r)r^2dr\ . \quad (4.11)$$

In the OCP the bare electric field $\epsilon(r)$ is of the $1/r^2$ form. In our plasmas $\epsilon(r)$ has a more complicated form and cannot be approximated by a Debye-like form. Nevertheless, to implement a form of APEX we assume that $\epsilon(r)$ arises from a Debye-like potential $V_\epsilon(r)=e^{-\lambda r}/r$, where λ has to be determined by fitting to our electric fields. The effective field $\epsilon^*(r)$ appearing in (4.10) is assumed to arise from a potential $e^{-(\lambda+\alpha)r}$, where α is the adjustable parameter of APEX. Thus

$$\epsilon^*(r)=\epsilon(r)\left[\frac{1+(\lambda+\alpha)r}{1+\lambda r}\right]e^{-\alpha r}\ . \quad (4.12)$$

Fitting the numerical data for the (deconvoluted plasma model) electric field $\epsilon(r)$ in the hydrogen plasma, we find that

$$\lambda=\begin{cases}\lambda_D^e, & \text{for } r\sim 2 \text{ or } 3 \text{ a.u.}\\ 1.5\lambda_D^e, & \text{for } r\sim 5 \text{ a.u.}\end{cases}$$

where λ_D^e is the electron Debye screening constant. Hence we have made two APEX calculations, viz., APEX1 and APEX2 with $\lambda=\lambda_D^e$ and $\lambda=1.5\lambda_D^e$, respectively. For each choice of λ, a value of α is obtained by requiring that $T_2^{\rm BM}=T_2^{\rm APEX}$, from Eqs. (4.10) and (4.11). Since the choices $\lambda=\lambda_D^e$ or $1.5\lambda_D^e$ both fail in some regions of r in fitting $\epsilon(r)$, all that we can hope for is that these two calculations give an indication of what the APEX estimate of $\Delta W_\infty^{\rm APEX}$ would be. It is interesting to note that the term $\Delta h_{pp}^a=h_{pp}^2-(h_{pp}^0)^2$, given more explicitly in Eq. (2.30), does not change the coefficient T_2^{BM}, i.e., does not change the second moment $\langle\epsilon^2\rangle$. This can be verified by noting that the contribution to T_2, viz., ΔT_2 from the *ipp* correction is given by

$$\tfrac{1}{2}\bar{\rho}^2\{g_{ip}(0,1)[i\mathbf{r}_2\cdot\boldsymbol{\epsilon}(0,1)]h_{ip}(0,1)d\mathbf{r}_1\}^2 - \tfrac{1}{2}\bar{\rho}^2\{g_{ip}(0,1)[i\mathbf{r}_2\cdot\boldsymbol{\epsilon}(0,1)]h_{pp}(0,1)d\mathbf{r}_1\}^2\ .$$

This correction vanishes by its angular part $\int_0^\pi\cos\theta\sin\theta d\theta$. The dominant effects of the *ipp* correction appear in x^4 and beyond, and hence cannot be captured by the APEX method. In this context we note that, to order x^2, APEX involves a physical model where the interacting plasma is replaced by an effective noninteracting plasma, i.e., only the impurity-plasma interactions remain. (Note that in the OCP, or in a homogeneous plasma, the *ipp* correction is zero.) Hence any modification of plasma-plasma correlation via the impurity should not contribute, as was explicitly found to be the case.

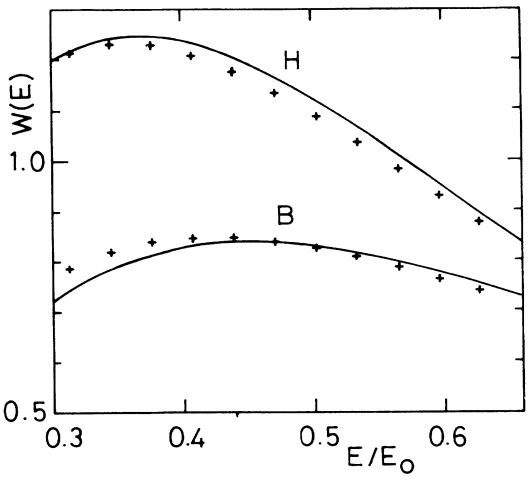

FIG. 7. All-order microfield distributions [$W_\infty(E)$ without *ipp* corrections] for H and B impurities. Full curve: WCS calculation; crosses: APEX1, i.e., $\lambda=\lambda_D^e$ with the electric field from Δn_p of the deconvoluted plasma model.

Numerical results of ΔW_∞ obtained from APEX1, APEX2 and WCS are given in Table V (see also Fig. 7). It is seen that APEX2 with $\lambda=1.5\lambda_D^e$ (compared with APEX1 where $\lambda=\lambda_D^e$) gives a somewhat larger correction for larger fields. WCS also behaves in a similar way, but the differences from APEX1 are more pronounced. The all-order estimate given by WCS is seen to be smaller than the APEX estimates, although essentially in the same direction. It should be noted that, unlike the case of pure Coulomb interactions, the APEX, as it is used here, is somewhat weakened by the lack of an exact sum rule. Sensitivity to deviations from the sum rule could be modeled by deviations of α from the optimal value. In our calculations we have, in fact, given two different APEX calculations. It is seen from Table V that APEX1 and APEX2 are close to each other in comparison to the difference between the mean of APEX1 and APEX2 and the WCS calculation. Hence, based on the OCP comparison between APEX and WCS established in Ref. 5, it is rather surprising that the two methods do not agree more closely. This shows that the theory of all-order summations for electron-ion plasmas needs further improvement, particularly when ions having internal structure need to be considered.

V. CONCLUDING SUMMARY

In this paper we have achieved the following: (i) shown how an impurity placed in a plasma effects the plasma-plasma pair correlations, and clarified the relationship of the two-component plasma models and inhomogeneous plasma models which have been used for studying this problem; (ii) discussed how the electric field due to an individual ion in a dense plasma could be defined without using a "uniform jellium background" assumption; (iii) evaluated the effect of these two corrections on the second-order Baranger-Mozer microfield probability distributions at He, Li, Be, and B impurities in a hydrogen plasma; and (iv) evaluated the contribution to the microfield probability distribution beyond second order using two versions of APEX and also the WCS method; (v) given a new treatment of the impurity-plasma modeling of the fractional quantum Hall effect excitations. We conclude that an evaluation of the BM second-order microfield distribution inclusive of all the relevant corrections is now possible, but the evaluation of the all-order contributions needs to be improved, especially in dealing with electron-ion plasmas, where the electron-ion coupling is not weak.

ACKNOWLEDGMENTS

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[1]See, H. R. Griem, *Spectral Line Broadening by Plasma* (Academic, New York, 1974). Also see J. W. Dufty, in *Strongly Coupled Plasma Physics,* edited by F. J. Rogers and H. E. DeWitt (Plenum, New York, 1986), p. 493.

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[14]See Fig. 1 of F. Perrot and M. W. C. Dharma-wardana, Phys. Rev. A **29**, 1378 (1984), where bound states in hydogen plasmas in the $\Gamma=0.1$ to $10r_s=1,2$ have been discussed. See also Table I of Ref. 4, where the structure of an Al ion in a hydrogen plasma has been studied.