

## Interpretation of positron-annihilation data with respect to the electron-positron enhancement factors. I. Theory

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(Received 7 August 1992)

The influence of the positron distribution and electron-positron interactions on the momentum density  $\rho(\mathbf{p})$  of annihilation quanta in real metals is discussed on mathematical grounds. We show that in simple metals, neither the assumed form of the positron wave function nor state-independent electron-positron correlations can change appreciably the shape of  $\rho(\mathbf{p})$  inside the central Fermi surface. The role of momentum dependence of two-particle correlations is set forth. For localized electronic populations, this property does not occur: both the form of the positron distribution and the locality of correlation effects have a crucial influence on the resulting momentum density  $\rho(\mathbf{p})$ . The same features have the umklapp components for delocalized electrons.

### I. INTRODUCTION

The angular correlation of positron  $2\gamma$  annihilation radiation (ACPAR) technique has been established for studies of the electronic structure of materials, particularly for electron momentum spectroscopy.<sup>1</sup> In solids, however, due to strong electron-positron correlations as well as to the deviation of the positron distribution from the uniform one, the electron momentum density (EMD) in the material investigated,  $\rho^e(\mathbf{p})$ , differs from the momentum density of the  $2\gamma$  annihilation quanta  $\rho^{2\gamma}(\mathbf{p})$  (whose one- and two-dimensional projections are provided by the ACPAR experiment) by a factor  $\epsilon^{2\gamma}(\mathbf{p}) = \rho^{2\gamma}(\mathbf{p})/\rho^e(\mathbf{p})$ . In the present work we focus our attention on the momentum dependence of this function.

Recently there have been theoretical studies of the influence of the positron distribution in the lattice on the resulting positron-annihilation characteristics.<sup>2</sup> This effect is well described by the function  $\epsilon^{\text{IPM}}(\mathbf{p}) = \rho^{\text{IPM}}(\mathbf{p})/\rho^e(\mathbf{p})$ , where  $\rho^{\text{IPM}}$  is the momentum density obtained within the independent particles model (IPM). The features of  $\epsilon^{\text{IPM}}(\mathbf{p})$  and  $\epsilon^{2\gamma}(\mathbf{p})$  for electronic populations of various degree of localization are discussed on mathematical grounds in Secs. II and III of this work.

A series of papers in the field is devoted to determining enhancement factors  $\epsilon^{\text{corr}}(\mathbf{p}) = \rho^{2\gamma}(\mathbf{p})/\rho^{\text{IPM}}(\mathbf{p})$  in jellium,<sup>3</sup> in real metals,<sup>4-8</sup> as well as from experiment.<sup>9</sup> This function provides information about electron-positron correlations (cf. Sec. II). The role of the momentum selectivity of two-particle electron-positron correlation functions is discussed in Sec. III.

In theoretical calculations of  $\rho^{2\gamma}(\mathbf{p})$  [or  $\epsilon^{\text{corr}}(\mathbf{p})$ ] in real metals various approximations to electron-positron interaction effects have been used. One group of papers is based on the ladder approximation to the electron-positron Green's function.<sup>4</sup> Other approaches use the average electron density<sup>5</sup> (AED) or local-density approximations<sup>6-8</sup> (LDA), both based on the results for  $\epsilon_{\text{jell}}^{\text{corr}}(p, r_s)$  obtained within the jellium model<sup>3</sup> for various electron density parameters  $r_s$ . In Sec. III we show on

mathematical grounds that for nearly parabolic electronic bands  $j$ , results for correlation factors  $\epsilon^{\text{corr}}(\mathbf{p})$  are very close to corresponding characteristics obtained within the AED.<sup>5</sup> Practical applications of this result are presented in Ref. 10 (paper II of this work), where the electron density parameters describing correlation effects for valence electrons in simple metals are calculated within the LDA.

According to recent theoretical and experimental works,<sup>8(b),7(c)</sup> for more localized electronic populations the influence of the positron model on the resulting shape of  $\epsilon^{\text{corr}}(\mathbf{p})$  is not negligible. This fact is in agreement with expectations: for more localized electrons, the nonuniform positron distribution changes the shape of  $\rho^{\text{IPM}}(\mathbf{p})$  and therefore  $\epsilon^{\text{corr}}(\mathbf{p})$ . In contrast to the "experimental" factor  $\epsilon_{\text{expt}}^{\text{corr}}(\mathbf{p})$  as well as theoretical ones  $\epsilon^{2\gamma}(\mathbf{p})$ ,  $\epsilon^{\text{corr}}(\mathbf{p})$ , and  $\epsilon^{\text{IPM}}(\mathbf{p})$ , the experimental characteristic  $\epsilon_{\text{expt}}^{2\gamma}(\mathbf{p}) = \rho_{\text{expt}}^{2\gamma}(\mathbf{p})/\rho^e(\mathbf{p})$  does not depend on the assumptions about the positron wave function. For this reason  $\epsilon_{\text{expt}}^{2\gamma}(\mathbf{p})$  seems to be more reliable than  $\epsilon_{\text{expt}}^{\text{corr}}(\mathbf{p})$  and we would like to recommend it here. It should be noted here that in a series of experimental works [cf., e.g., Refs. 7(b), 8(b), and 8(d) of Ref. 10] as well as in theoretical calculations for jellium,  $\epsilon^{\text{corr}}$  is in practice replaced by  $\epsilon^{2\gamma}$ , according to the assumption  $\epsilon^{\text{IPM}}(\mathbf{p}) = 1$  [or  $\rho^{\text{IPM}}(\mathbf{p}) = \Theta(E_F - E_p)$ , where  $\Theta$  and  $E_F$  are the Heaviside step function and Fermi energy, respectively]. In Ref. 10 we discuss the methods of determining  $\epsilon_{\text{expt}}^{\text{corr}}(\mathbf{p})$  from "coarse" positron-annihilation data.

### II. BASIC FORMULAS

The EMD, which is an important characteristic of the electronic structure in the material investigated, is given by the formula

$$\begin{aligned} \rho^e(\mathbf{p}) &= \frac{1}{\Omega} (-i)^2 \int_{\Omega} \int_{\Omega} e^{-i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}_1)} G_e(\mathbf{r}\mathbf{t}; \mathbf{r}_1\mathbf{t}^+) d\mathbf{r} d\mathbf{r}_1 \\ &= \frac{1}{\Omega} \sum_i n(i) \left| \int_{\Omega} e^{-i\mathbf{p}\cdot\mathbf{r}} \psi_i^e(\mathbf{r}) d\mathbf{r} \right|^2, \end{aligned} \quad (1)$$

where  $\Omega$  is the volume of the unit cell and  $n(i)$  denotes the occupation number of the electronic state  $i$ .  $G_e$  and  $\psi_i^e$  are the electron Green's and wave functions, respectively.

Positron-annihilation apparatus measures one- or two-dimensional (1D or 2D, respectively) momentum probability distributions

$$N(p_z) = \frac{1}{\lambda} \int \int dp_x dp_y \rho^{2\gamma}(\mathbf{p}) \quad (2a)$$

and

$$N(p_x, p_z) = \frac{1}{\lambda} \int dp_y \rho^{2\gamma}(\mathbf{p}). \quad (2b)$$

The unnormalized momentum density of the  $2\gamma$  annihilation quanta (partial annihilation rate) is given by the formula [cf., e.g., Refs. 1(c) and 3(b)]

$$\begin{aligned} \rho^{2\gamma}(\mathbf{p}) &= \frac{\pi r_0^2 c}{\Omega} (-i)^2 \int_{\Omega} \int_{\Omega} e^{-i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}_1)} G_{ep}(\mathbf{r}t, \mathbf{r}t; \mathbf{r}_1 t^+, \mathbf{r}_1 t^+) d\mathbf{r} d\mathbf{r}_1 \\ &= \frac{\pi r_0^2 c}{\Omega} \sum_i n(i) \left| \int_{\Omega} e^{-i\mathbf{p}\cdot\mathbf{r}} \psi_i^e(\mathbf{r}) \left[ \psi_+(\mathbf{r}) \frac{\psi_i^{ep}(\mathbf{r}, \mathbf{r})}{\psi_i^e(\mathbf{r}) \cdot \psi_+(\mathbf{r})} \right] d\mathbf{r} \right|^2, \end{aligned} \quad (3a)$$

where  $r_0$  and  $c$  are the classical electron radius and velocity of light, respectively. The constant which normalizes  $N(p_z)$  and  $N(p_x, p_z)$ ,

$$\begin{aligned} \lambda &= \int \rho^{2\gamma}(\mathbf{p}) d\mathbf{p} = \pi r_0^2 c (-i)^2 \int_{\Omega} d\mathbf{r} G_{ep}(\mathbf{r}t, \mathbf{r}t; \mathbf{r}t^+, \mathbf{r}t^+) \\ &= \pi r_0^2 c \int_{\Omega} d\mathbf{r} |\psi_+(\mathbf{r})|^2 \left[ \sum_i n(i) |\psi_i^e(\mathbf{r})|^2 \left| \frac{\psi_i^{ep}(\mathbf{r}, \mathbf{r})}{\psi_i^e(\mathbf{r}) \cdot \psi_+(\mathbf{r})} \right|^2 \right], \end{aligned} \quad (3b)$$

is the total annihilation rate related to the positron lifetime  $\tau$  as  $\lambda = 1/\tau$ .  $G_{ep}$  in Eqs. (3a) and (3b) is the zero-temperature electron-positron Green's function,  $\psi_i^{ep}(\mathbf{r}_e, \mathbf{r}_p)$  denotes the pair wave function of the electron in the initial state  $i$  located at  $\mathbf{r}_e$  and thermalized positron at  $\mathbf{r}_p$ , and  $\psi_+$  is the positron wave function.

The quantity  $\rho^{2\gamma}(\mathbf{p})$ , which can be determined by ACPAR, differs from the EMD by a momentum-dependent factor

$$\varepsilon^{2\gamma}(\mathbf{p}) = \rho^{2\gamma}(\mathbf{p}) / \rho^e(\mathbf{p}). \quad (3c)$$

For this reason, in practical applications of ACPAR data to investigations of the electronic structure of solids, first of all the knowledge of  $\varepsilon^{2\gamma}(\mathbf{p})$  is necessary.

In quite a few works the studies of  $\rho^{2\gamma}(\mathbf{p})$  are limited to the IPM. Within the IPM electron-positron correlations are neglected, i.e., one assumes  $\psi_i^{ep}(\mathbf{r}_e, \mathbf{r}_p) = \psi_i^e(\mathbf{r}_e) \psi_+(\mathbf{r}_p)$  ( $G_{ep} = G_e G_p$ ). In this case Eq. (3a) leads to well-known IPM ACPAR formula

$$\rho^{\text{IPM}}(\mathbf{p}) = \frac{\pi r_0^2 c}{\Omega} \sum_i n(i) \left| \int_{\Omega} e^{-i\mathbf{p}\cdot\mathbf{r}} \psi_i^e(\mathbf{r}) \cdot \psi_+(\mathbf{r}) d\mathbf{r} \right|^2, \quad (4a)$$

The corresponding factor

$$\varepsilon^{\text{IPM}}(\mathbf{p}) = \rho^{\text{IPM}}(\mathbf{p}) / \rho^e(\mathbf{p}) \quad (4b)$$

and the IPM annihilation rate

$$\begin{aligned} \lambda^{\text{IPM}} &= \int \rho^{\text{IPM}}(\mathbf{p}) d\mathbf{p} \\ &= \pi r_0^2 c \int_{\Omega} d\mathbf{r} |\psi_+(\mathbf{r})|^2 \sum_i n(i) |\psi_i^e(\mathbf{r})|^2 \end{aligned} \quad (4c)$$

provide information about the influence of the shape of the positron wave function on the resulting ACPAR spectrum [cf., e.g., Refs. 2, 6(d), 6(e), and 11] and positron lifetime.<sup>8</sup>

The function  $\varepsilon^{2\gamma}(\mathbf{p})$  reads as the product of  $\varepsilon^{\text{corr}}(\mathbf{p})$  and  $\varepsilon^{\text{IPM}}(\mathbf{p})$ . The enhancement factors (most often investigated in theoretical and experimental works)

$$\varepsilon^{\text{corr}}(\mathbf{p}) = \rho^{2\gamma}(\mathbf{p}) / \rho^{\text{IPM}}(\mathbf{p}) \quad (5a)$$

and

$$\gamma^{\text{corr}} = \lambda / \lambda^{\text{IPM}} \quad (5b)$$

describe electron-positron correlation effects, as schematically shown in Fig. 1. It should be stressed here that due to normalization constant  $\lambda$  appearing in formulas (2a) and (2b) for experimental curves  $N(p_z)$  or  $N(p_x, p_z)$ , neither  $\varepsilon_{\text{expt}}^{2\gamma}(\mathbf{p}=\mathbf{0})$  nor  $\varepsilon_{\text{expt}}^{\text{corr}}(\mathbf{p}=\mathbf{0})$  are extractable directly from 1D or 2D ACPAR data. The only available functions are  $\varepsilon_{\text{expt}}^{2\gamma}(\mathbf{p}) / \varepsilon_{\text{expt}}^{2\gamma}(\mathbf{0})$  and  $\varepsilon_{\text{expt}}^{\text{corr}}(\mathbf{p}) / \varepsilon_{\text{expt}}^{\text{corr}}(\mathbf{0})$  [cf. also

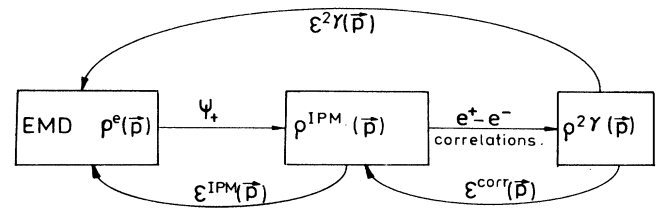


FIG. 1. Scheme of relation between EMD and studied momentum density of annihilation pairs.

Eq. (3)]. The quantities  $\varepsilon_{\text{expt}}^{2\gamma}(\mathbf{0})$  and  $\varepsilon_{\text{expt}}^{\text{corr}}(\mathbf{0})$  may be determined if the positron lifetime  $\tau = 1/\lambda$  is known together with the full shape of the ACPAR spectrum.

Positron and unperturbed electron wave functions (Green's functions) used in Eqs. (1), (3), and (4) may be obtained within standard band-structure calculations. It is not so with functions  $\psi_i^{ep}$  (or  $G_{ep}$ ) of Eqs. (3a) and (3b). For determining  $G_{ep}$  or the respective correlation factors

$$f_i(\mathbf{r}) = |\psi_i^{ep}(\mathbf{r}, \mathbf{r})|^2 / |\psi_i^e(\mathbf{r})\psi_+(\mathbf{r})|^2, \quad (6)$$

in real metals, various approximations have been used, leading to alternative results for  $\varepsilon^{\text{corr}}(\mathbf{p})$  (Refs. 4–7) and  $\lambda$  (Ref. 8). Of particular interest is the LDA developed in a series of papers.<sup>6–8</sup> Within the LDA the functions  $f_i(\mathbf{r})$  are approximated by correlation functions in jellium of local electron density characterized by the parameter  $r_s(\mathbf{r})$ , i.e.,

$$f_i^{\text{LDA}}(\mathbf{r}) = \varepsilon_{\text{jell}}^{\text{corr}}[\kappa(E_i, \mathbf{r}), r_s(\mathbf{r})], \quad (7)$$

where  $E_i$  is the energy of the initial electronic state  $i$  and  $\kappa$  is chosen in various papers in different ways.

It should be noted here that, if within the LDA,  $f_i(\mathbf{r})$  is assumed to be independent of  $\mathbf{r}$  [i.e.,  $f_i^{\text{LDA}}(\mathbf{r})$  is approximated by  $\varepsilon_{\text{jell}}^{\text{corr}}(E_i, r_s^*)$ , where  $r_s^*$  is some effective electron density parameter], the approach reduces to the average density approximation<sup>5</sup>

$$\rho_{\text{AED}}^{2\gamma}(\mathbf{p}) = \sum_{\mathbf{k}j} \varepsilon_{\text{jell}}^{\text{corr}}(E_{\mathbf{k}j}, r_s^*) \rho^{\text{IPM}}(\mathbf{p}), \quad (8)$$

where  $\mathbf{k}$  and  $j$  are the electron momentum in the reduced zone scheme and band number, respectively, and momentum  $\mathbf{p}$  represents  $\mathbf{k}$  in the extended zone scheme. When the state selectivity of  $f_i(\mathbf{r})$  is neglected [i.e.,  $f_i(\mathbf{r}) \equiv g(\mathbf{r})$ ], as in Ref. 7, we get

$$\rho^{2\gamma}(\mathbf{p}) = \alpha \cdot \rho_1^{\text{IPM}}(\mathbf{p}),$$

where  $\rho_1^{\text{IPM}}(\mathbf{p})$  is the IPM momentum density obtained according to Eq. (4a) with *another* positron wave function  $\psi_+^1(\mathbf{r}) = \psi_+(\mathbf{r})g(\mathbf{r})^{1/2}\alpha^{-1/2}$  [the normalization constant  $\alpha$  is equal to  $\int g(\mathbf{r})|\psi_+(\mathbf{r})|^2 d\mathbf{r}$ ]. The enhancement factor  $\varepsilon^{2\gamma}(\mathbf{p})$  reduces in this case to an IPM one,  $\alpha\varepsilon_1^{\text{IPM}}(\mathbf{p})$ , for a positron wave function  $\psi_+^1(\mathbf{r})$ . In an electron gas, characterized by  $r_s(\mathbf{r}) \equiv r_s^*$ , this approximation leads to the momentum density of the IPM shape, i.e.,  $\rho^{2\gamma}(\mathbf{p}) = \alpha\rho^{\text{IPM}}(\mathbf{p})$ , giving  $\varepsilon^{\text{corr}}(\mathbf{p}) = \alpha$ . For delocalized electronic populations in real metals the same feature occurs for momenta  $\mathbf{p}$  less than the Fermi momentum  $p_F$ ,<sup>6(d),6(e),11</sup> as proved in Sec. III. This behavior of  $\rho^{2\gamma}(\mathbf{p})$  shows that a great deal of caution is necessary when the dependence of two-particle electron-positron correlations on the initial electronic state is neglected in the ACPAR formula (3a).

### III. ELECTRON-POSITRON ENHANCEMENT FACTORS FOR VARIOUS ELECTRON POPULATIONS

In this section the influence of the positron distribution as well as of the local correlation effects  $f_i(\mathbf{r})$  on the resulting momentum density  $\rho^{2\gamma}(\mathbf{p})$  is discussed. Let us

take into account the contribution of  $j$ th band of electronic Bloch states

$$\psi_{\mathbf{k}j}^e(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}\cdot\mathbf{r}} \left[ \sum_{\mathbf{G}} u_{\mathbf{k}j}(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}} \right] \quad (9a)$$

to the EMD and  $\rho^{2\gamma}(\mathbf{p})$ . Here  $\mathbf{G}$  denote the reciprocal lattice vectors, and momenta  $\mathbf{k}$  are in the first Brillouin zone (1BZ).

Due to normalization of  $\psi_{\mathbf{k}j}^e(\mathbf{r})$ , coefficients  $u_{\mathbf{k}j}$  satisfy the equation

$$\sum_{\mathbf{G}} |u_{\mathbf{k}j}(\mathbf{G})|^2 = 1. \quad (9b)$$

Let us mention here that for any chosen state  $\mathbf{k}j$  there exists at least one reciprocal lattice vector  $\mathbf{G}_{\mathbf{k}j}$  such that  $|u_{\mathbf{k}j}(\mathbf{G}_{\mathbf{k}j})| \geq |u_{\mathbf{k}j}(\mathbf{G})|$ . Moreover, for any fixed momentum  $\mathbf{p}$  in the extended zone scheme (i.e., fixed  $\mathbf{G}^*$ , such that  $\mathbf{k} = \mathbf{p} - \mathbf{G}^* \in 1\text{BZ}$ ) there is at least one state  $\mathbf{k}j^*$  such that

$$|u_{\mathbf{k}j^*}(\mathbf{G}^*)| \geq |u_{\mathbf{k}j}(\mathbf{G}^*)|.$$

For our analysis of annihilation characteristic it is convenient to check how the electronic density for momentum  $\mathbf{p}$ ,

$$\begin{aligned} \rho^e(\mathbf{p} = \mathbf{k} + \mathbf{G}^*) &= \sum_j n(\mathbf{k}j) |u_{\mathbf{k}j}(\mathbf{G}^*)|^2 \\ &= |u_{\mathbf{k}j^*}(\mathbf{G}^*)|^2 \\ &\quad \times \left[ n(\mathbf{k}j^*) + \sum_{j \neq j^*} n(\mathbf{k}j) \left| \frac{u_{\mathbf{k}j}(\mathbf{G}^*)}{u_{\mathbf{k}j^*}(\mathbf{G}^*)} \right|^2 \right], \end{aligned} \quad (10)$$

changes after perturbing functions  $\psi_{\mathbf{k}j}^e$  by the corresponding functions

$$\chi_{\mathbf{k}j}(\mathbf{r}) = \psi_{\mathbf{k}j}^{ep}(\mathbf{r}, \mathbf{r}) / \psi_{\mathbf{k}j}^e(\mathbf{r}) = \psi_+(\mathbf{r}) [f_{\mathbf{k}j}(\mathbf{r})]^{1/2}. \quad (11a)$$

The correlation functions  $f_{\mathbf{k}j}(\mathbf{r})$ , given by Eq. (6), and the positron wave function  $\psi_+(\mathbf{r})$  are periodic in the lattice. Thus the functions  $\chi_{\mathbf{k}j}(\mathbf{r})$  are also periodic<sup>12</sup> and they may be expanded into the Fourier series with respect to reciprocal lattice vectors  $\mathbf{G}$ , i.e.,

$$\chi_{\mathbf{k}j}(\mathbf{r}) = \sum_{\mathbf{G}} h_{\mathbf{k}j}(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}}. \quad (11b)$$

We would like to stress here that, except for the IPM case,  $\chi_{\mathbf{k}j}$  should not be understood as the wave functions; beyond the IPM  $\chi_{\mathbf{k}j}(\mathbf{r})$  is not normalized to unity, due to correlation effects. Also the function  $\psi_{\mathbf{k}j}^{ep}(\mathbf{r}, \mathbf{r})$ , treated as a function of *only one* variable  $\mathbf{r}$ , cannot be considered as the eigenfunction of *any* one-particle Schrödinger equation, as was assumed incorrectly by Yongming *et al.*<sup>13</sup> Indices  $(\mathbf{k}j)$  in  $\chi_{\mathbf{k}j}(\mathbf{r})$  are referred to the *initial electronic states* in the host material.

Introducing  $\chi_{\mathbf{k}j}(\mathbf{r})$  we generalize the problem presented in the preceding section: if  $\chi_{\mathbf{k}j}$  is approximated by the positron wave function  $\psi_+(\mathbf{r})$  [ $f_{\mathbf{k}j}(\mathbf{r})$  is assumed to be equal to 1], we study the density  $\rho^{\text{IPM}}(\mathbf{p})$ ; for

$\chi_{kj}(\mathbf{r}) = \psi_+(\mathbf{r}) [g(\mathbf{r})]^{1/2}$  [ $f_{kj}(\mathbf{r})$  does not depend on  $\mathbf{k}j$ ] we have the case of state-independent correlations used in several works;<sup>6-8</sup> if no approximations to  $\chi_{kj}(\mathbf{r})$  [ $f_{kj}(\mathbf{r})$ ] are made [cf. the expression in square brackets on the right-hand side of Eq. (3a)] we get exactly  $\rho^{2\gamma}(\mathbf{p})$ . It should be noted here that this formalism goes beyond the LDA, as, in general, no assumptions about the functions  $\chi_{kj}(\mathbf{r})$  [ $f_{kj}(\mathbf{r})$ ], except their periodicity, are made. In practice, however, the pair correlation functions

$$f_{kj}(\mathbf{r}) = \sum_{\mathbf{G}} F_{kj}(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}} \quad (11c)$$

behave regularly with respect to the electron density

$$n_{el}(\mathbf{r}) = \sum_i n(i) |\psi_i^e(\mathbf{r})|^2 = \sum_{\mathbf{G}} N_{el}(\mathbf{G}) e^{i\mathbf{G}\cdot\mathbf{r}}, \quad (11d)$$

i.e.,  $|\nabla_r f(\mathbf{r})| \leq \text{const} |\nabla_r n_{el}(\mathbf{r})|$  for any  $\mathbf{r}$  in the unit cell or, alternatively,  $|F_{kj}(\mathbf{G})/F_{kj}(\mathbf{0})|$

$\leq \text{const} |N_{el}(\mathbf{G})/N_{el}(\mathbf{0})|$  for any  $\mathbf{G} \neq \mathbf{0}$ . Moreover (see the Appendix),

$$\chi_{kj}(\mathbf{r}=\mathbf{0}) = 0.$$

According to Eqs. (3a), (6), (9a), and (11b), we can define the "generalized" momentum density  $\rho(\mathbf{p}=\mathbf{k}+\mathbf{G}^*)$  (cf. also theorem on the convolution),

$$\begin{aligned} \rho(\mathbf{k}+\mathbf{G}^*) &= \sum_j n(\mathbf{k}j) \left| \sum_{\mathbf{H}} u_{kj}(\mathbf{H}) h_{kj}(\mathbf{G}^*-\mathbf{H}) \right|^2 \\ &= \sum_j n(\mathbf{k}j) |u_{kj}(\mathbf{G}_{kj})|^2 \\ &\quad \times |h_{kj}(\mathbf{G}^*-\mathbf{G}_{kj})|^2 |1+\alpha(\mathbf{k}j, \mathbf{G}^*)|^2 \end{aligned} \quad (12a)$$

where  $\mathbf{H}$  denote the reciprocal lattice vectors, and the functions

$$\alpha(\mathbf{k}j, \mathbf{G}^*) = [h_{kj}(\mathbf{G}^*-\mathbf{G}_{kj})]^{-1} \sum_{\mathbf{H} \neq \mathbf{G}_{kj}} h_{kj}(\mathbf{G}^*-\mathbf{H}) \frac{u_{kj}(\mathbf{H})}{u_{kj}(\mathbf{G}_{kj})} \quad (12b)$$

are dependent on the initial electronic state  $\mathbf{k}j$  (through  $u_{kj}$ ) and may take positive or negative values, depending on the band number  $j$  and reciprocal lattice vector  $\mathbf{G}^*$ . The constant  $\pi r_0^2 c$ , appearing in the definitions of  $\rho^{2\gamma}(\mathbf{p})$  [Eq. (3a)] and  $\rho^{\text{IPM}}(\mathbf{p})$  [Eq. (4a)], is omitted in the formula (12a) for convenience.

Let us consider two cases: nearly free and localized electronic populations.

#### A. Nearly parabolic electronic bands

As follows from band-structure calculation results, the nearly free electron (NFE) model is quite reasonable, e.g., for valence electrons in simple metals (Al, Mg, and alkali metals). Except for the states close to the Brillouin-zone boundary, there is only one "leading" term in the Fourier representation of  $\psi_{kj}^e(\mathbf{r})$ ,  $|u_{kj}(\mathbf{G})|$ , and the other (umklapp) components are very small [cf. Eqs. (9a) and (9b)]. This means that for any chosen state  $\mathbf{k}j$  (excluding those on the BZ boundary) there is *only one* reciprocal lattice vector  $\mathbf{G}_{kj}$  such that

$$|u_{kj}(\mathbf{G}_{kj})| \gg |u_{kj}(\mathbf{G})| \quad \text{for } \mathbf{G} \neq \mathbf{G}_{kj}, \quad (13a)$$

and for any fixed momentum  $\mathbf{p}=\mathbf{k}+\mathbf{G}^*$  there is *only one* state  $\mathbf{k}j^*$  such that

$$|u_{kj^*}(\mathbf{G}^*)| \gg |u_{kj}(\mathbf{G}^*)| \quad \text{for } j \neq j^*. \quad (13b)$$

Relations (13a) and (13b) clearly imply that

$$\mathbf{G}_{kj^*} = \mathbf{G}^*, \quad \mathbf{G}_{kj} \neq \mathbf{G}^* \quad \text{for } j \neq j^*. \quad (13c)$$

For momenta  $\mathbf{p}$  inside the central Fermi surface (FS) the state  $(\mathbf{p}-\mathbf{G}^*, j^*)$  is occupied, while for  $\mathbf{p}$  outside the FS,  $n(\mathbf{p}-\mathbf{G}^*, j^*)=0$ .

We shall start our studies of  $\rho(\mathbf{p})$  and  $\varepsilon(\mathbf{p})$  for momenta  $\mathbf{p}$  inside the FS. For any fixed momentum  $\mathbf{p} \in \text{FS}$

$$n(\mathbf{k}=\mathbf{p}-\mathbf{G}^*, j^*) = 1. \quad (13d)$$

According to condition (13),  $\rho^e(\mathbf{p})$  [Eq. (10)] and  $\rho(\mathbf{p})$  [Eq. (12)] can be approximated by (cf. the Appendix)

$$\rho_{\text{NFE}}^e(\mathbf{p}=\mathbf{k}+\mathbf{G}^*) \cong |u_{kj^*}(\mathbf{G}^*)|^2 \quad (14a)$$

and

$$\rho_{\text{NFE}}(\mathbf{p}=\mathbf{k}+\mathbf{G}^*) \cong |u_{kj^*}(\mathbf{G}^*)|^2 |h_{kj^*}(\mathbf{0})|^2 \left[ 1 + \sum_{j \neq j^*} |\beta(\mathbf{k}j, \mathbf{G}^*)|^2 \right], \quad (14b)$$

where

$$\beta(\mathbf{k}j, \mathbf{G}^*) = n(\mathbf{k}j) \frac{h_{kj}(\mathbf{G}^*-\mathbf{G}_{kj})}{h_{kj}(\mathbf{0})} \frac{u_{kj}(\mathbf{G}_{kj})}{u_{kj^*}(\mathbf{G}^*)} \frac{h_{kj}(\mathbf{0})}{h_{kj^*}(\mathbf{0})}. \quad (14c)$$

Since the umklapp components of  $\rho_{\text{NFE}}^e(\mathbf{p})$  inside the FS are small, the contribution of one band dominates, i.e.,  $\rho_{\text{NFE}}^e(\mathbf{k} + \mathbf{G}^*) \cong \rho_{j^*}^e(\mathbf{k} + \mathbf{G}^*)$ .  $\rho_{\text{NFE}}^e(\mathbf{p})$  has similar properties, as shown below.

Equation (14b) is based on the assumption that, within NFE, functions  $\alpha(\mathbf{k}j^*, \mathbf{G}^*)$  and  $\alpha(\mathbf{k}j, \mathbf{G}^*)$  are negligible in comparison with unity. On the other hand, we should remember that although  $\alpha$  are very small, they are not exactly equal to zero in real NFE metals. These quantities, obtained within the LDA on the basis of band-structure calculation results, are presented for some of the simple metals in Ref. 10. As can be seen in Fig. 2 (cf. also Ref. 10), the approximation  $\alpha(\mathbf{k}j, \mathbf{G}^*) \cong 0$  is quite reasonable.

It should be noted here that if the whole FS is contained inside the 1BZ (as takes place, e.g., for all alkali metals), the only occupied band is  $j^* = 1$ , i.e.,  $n(\mathbf{k}j) = 0$  for  $j \neq j^*$ . In this case  $\rho_{\text{NFE}}^e(\mathbf{p})$  and the corresponding enhancement factor  $\epsilon(\mathbf{p})$  for  $\mathbf{p} \in \text{FS}$  reduce to  $(\mathbf{G}^* = \mathbf{0})$

$$\rho_{\text{NFE}}^e(\mathbf{p} = \mathbf{k}) \cong |u_{\mathbf{k}j^*}(\mathbf{0})|^2 |h_{\mathbf{k}j^*}(\mathbf{0})|^2 \quad (15a)$$

and

$$\epsilon_{\text{NFE}}(\mathbf{p} = \mathbf{k}) \cong |h_{\mathbf{k}j^*}(\mathbf{0})|^2. \quad (15b)$$

If the functions  $\chi_{\mathbf{k}j}(\mathbf{r})$  are independent of the electronic state  $\mathbf{k}j$  [the case of IPM (Ref. 2) and  $f_{\mathbf{k}j}(r) \cong g(r)$  (Ref

7)], i.e.,  $\chi_{\mathbf{k}j}(\mathbf{r}) = \chi(\mathbf{r})$ , the enhancement factor

$$\epsilon_{\text{NFE}}(\mathbf{p}) \cong |h(\mathbf{0})|^2 \quad (15c)$$

does not depend on the momentum either. This fact is illustrated in Fig. 2, where *two* relative enhancement factors  $\epsilon_{\text{val}}^{\text{IPM}}(\mathbf{p})/\epsilon_{\text{val}}^{\text{IPM}}(\mathbf{0})$  and  $\epsilon_{\text{val}}^{\text{corr}}(\mathbf{p})/\epsilon_{\text{val}}^{\text{corr}}(\mathbf{0})$ , obtained within the LDA for  $\chi_{\mathbf{k}j}$  independent of the electronic state  $\mathbf{k}j$ , calculated for valence electrons in Na are presented by a *one* dashed line. It should be noted here that our theoretical considerations deal with  $\epsilon^{\text{IPM}}(\mathbf{p})$  and  $\epsilon^{2\gamma}(\mathbf{p}) = \epsilon^{\text{IPM}}(\mathbf{p})\epsilon^{\text{corr}}(\mathbf{p})$  only, because both these quantities describe the change of the momentum density with respect to EMD. Since within NFE EMD and IPM momentum density have the same form inside the FS, i.e.,  $\rho_{\text{NFE}}^{\text{IPM}}(\mathbf{p})$  differs from  $\rho_{\text{NFE}}^e(\mathbf{p})$  by a constant factor  $|\psi_+(\mathbf{G} = \mathbf{0})|^2$  [cf. Eq. (15a)], the features of the corresponding correlation enhancement factor  $\epsilon_{\text{NFE}}^{\text{corr}}(\mathbf{p})$  may be identified with properties of  $\epsilon_{\text{NFE}}^{2\gamma}(\mathbf{p})$ .

It should be noted here that, as explained in Sec. II, the relative enhancement factor  $\epsilon(\mathbf{p})/\epsilon(\mathbf{0})$  only is extractable from experiment. In our case  $\epsilon_{\text{NFE}}(\mathbf{p})/\epsilon_{\text{NFE}}(\mathbf{0}) \cong 1$  up to the Fermi momentum. For this reason studies of influence of the shape of the positron wave function or state-independent correlations on the resulting shape of ACPAR spectrum for valence electrons in alkalis do not seem to be very instructive.

Let us consider the NFE metals in which the Fermi momentum is outside the 1BZ (cf., e.g., Al and Mg). It should be noted here that for correlation functions  $f_{\mathbf{k}j}(\mathbf{r})$  which behave regularly with respect to the electron density, i.e., for  $|F_{\mathbf{k}j}(\mathbf{G})/F_{\mathbf{k}j}(\mathbf{0})| \leq \text{const} |N_{el}(\mathbf{G})/N_{el}(\mathbf{0})|$  [this case includes IPM and LDA; cf. Eq. (7)], we have

$$|h_{\mathbf{k}j}^{\text{LDA}}(\mathbf{0})| \gg |h_{\mathbf{k}j}^{\text{LDA}}(\mathbf{G} \neq \mathbf{0})|, \quad (16a)$$

$$|u_{\mathbf{k}j}(\mathbf{G}_{\mathbf{k}j})|/|u_{\mathbf{k}j^*}(\mathbf{G}^*)| \cong 1,$$

and

$$|h_{\mathbf{k}j}^{\text{LDA}}(\mathbf{0})|^2/|h_{\mathbf{k}j^*}^{\text{LDA}}(\mathbf{0})|^2 < 2$$

for any  $\mathbf{k}, j$ , and  $j^*$  [according to any of calculations performed for jellium,<sup>3</sup>  $\epsilon_{\text{jell}}^{\text{corr}}(p_F)/\epsilon_{\text{jell}}^{\text{corr}}(\mathbf{0}) < 2$ ]. In this case the factors  $\beta(\mathbf{k}j, \mathbf{G}^*)$  in sum over  $j \neq j^*$  on the right-hand side of Eq. (14b) are small and the whole sum can be neglected. The corresponding momentum density and enhancement factor are given by

$$\rho_{\text{NFE}}^e(\mathbf{p} = \mathbf{k} + \mathbf{G}^*) \cong |u_{\mathbf{k}j^*}(\mathbf{G}^*)|^2 |h_{\mathbf{k}j^*}(\mathbf{0})|^2 \quad (16b)$$

and Eq. (15b), respectively. So, remarks concerning momentum dependence of  $\epsilon(\mathbf{p})$  in alkali metals remain valid for Fermi momentum beyond the 1BZ (see enhancement factors in Mg presented in Fig. 2).

It should be stressed here that calculations of electronic structure in Na and Mg have been performed within linear-muffin-tin-orbitals-average-spheres approximation using self-consistent potential parameters.<sup>6(d),6(e)</sup> As can be seen, our general considerations are confirmed by practical applications of real band-structure results. The small deviations of  $\epsilon_{\text{val}}^{\text{IPM}}(\mathbf{p})$ ,  $\epsilon_{\text{val}}^{\text{corr}}(\mathbf{p})$ , and  $\epsilon_{\text{val}}^{2\gamma}(\mathbf{p})$  from a constant value, occurring at the BZ boundary in Mg, can

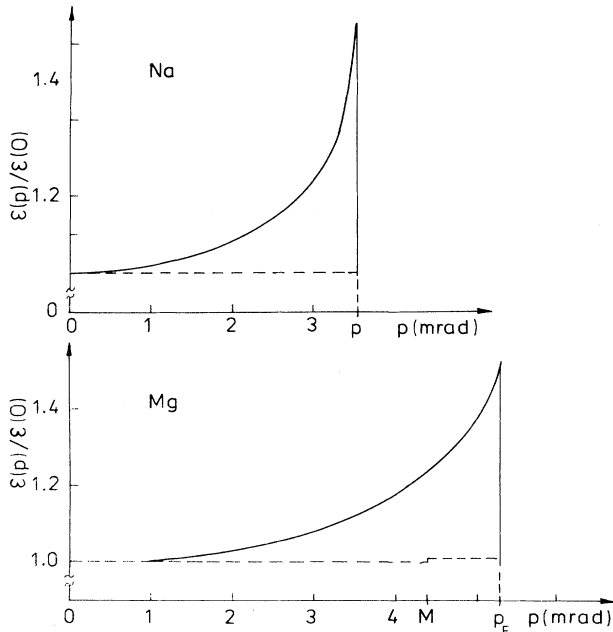


FIG. 2. Relative enhancement factors in Mg and Na inside the central Fermi surface.  $\epsilon^{\text{corr}}(\mathbf{p})$  obtained within LDA for  $f^{\text{LDA}}(r) = \epsilon_{\text{jell}}^{\text{corr}}[0, r_s(\mathbf{r})]$  and  $\epsilon_{\text{jell}}^{\text{corr}}[E_{\mathbf{k}j}, r_s(\mathbf{r})]$  are presented by dashed and solid lines, respectively.  $\epsilon^{\text{IPM}}(\mathbf{p})/\epsilon^{\text{IPM}}(\mathbf{0})$  is almost the same as state-independent  $\epsilon^{\text{corr}}(\mathbf{p})/\epsilon^{\text{corr}}(\mathbf{0})$ . The results are based on LMTO-ASA band-structure calculations [Refs. 6(d)–6(f)] where the values of  $\epsilon_{\text{jell}}^{\text{corr}}(p, r_s)$ , applied locally in  $f^{\text{LDA}}$ , were taken from Ref. 3(h).

be attributed to nonzero values of  $\beta(\mathbf{k}j, \mathbf{G}^*)$ , which change at this point. In Ref. 10 the effects coming from functions  $\alpha(\mathbf{k}j, \mathbf{G}^*)$  and  $\beta(\mathbf{k}j, \mathbf{G}^*)$  are discussed in detail.

As can be seen in Eqs. (15a), (15b), and (16b), the assumption on the state dependence of functions  $\chi_{\mathbf{k}j}(\mathbf{r})$  is of vital importance in studies of momentum density of annihilation quanta coming from nearly parabolic valence bands inside the FS. Neither  $\psi_+(\mathbf{r})$  (Ref. 2) nor

$$\begin{aligned} \epsilon_{\text{NFE}}^{\text{LDA}}(\mathbf{p}=\mathbf{k}+\mathbf{G}^*) &\cong \left| \int \{ \epsilon_{\text{jell}}^{\text{corr}}[\kappa(E_{\mathbf{k}j^*}/E_F, \mathbf{r}), r_s(\mathbf{r})] \}^{1/2} \psi_+(\mathbf{r}) d\mathbf{r} \right|^2 \\ &\cong \int \epsilon_{\text{jell}}^{\text{corr}}[\kappa(E_{\mathbf{k}j^*}/E_F, \mathbf{r}), r_s(\mathbf{r})] |\psi_+(\mathbf{r})|^2 d\mathbf{r}, \end{aligned}$$

which is similar to the expression

$$\epsilon_C(\mathbf{p}=\mathbf{k}+\mathbf{G}^*) = \int \epsilon_{\text{jell}}^{\text{corr}}[E_{\mathbf{k}j^*}/E_F, r_s(\mathbf{r})] |\psi_+(\mathbf{r})|^2 d\mathbf{r},$$

proposed by Chakraborty<sup>5(a)</sup> with AED. Here  $r_s(\mathbf{r}) = [4\pi \cdot n_{el}(\mathbf{r})/3]^{-1/3}$ . From the theorem on the average value for integrals we get

$$\epsilon_{\text{NFE}}^{\text{LDA}}(\mathbf{k}+\mathbf{G}^*) \cong \epsilon_{\text{jell}}^{\text{corr}}[E_{\mathbf{k}j^*}/E_F, r_s(\bar{\mathbf{r}})],$$

which for given momentum  $\mathbf{p}$  determines the effective electron density  $r_s^{\text{corr}} = r_s(\bar{\mathbf{r}})$ . The question is how far  $r_s(\bar{\mathbf{r}})$  is common for all momenta  $\mathbf{p}$  inside the FS and whether the corresponding factor  $\gamma^{\text{corr}}$  in real metals is equal to its analogs obtained within the model of jellium<sup>3</sup> of the same density  $\gamma_{\text{jell}}^{\text{corr}}[r_s(\bar{\mathbf{r}})]$ . If so, the AED would be a great advantage in the studies of EMD by positron annihilation; knowing only  $\lambda_{\text{val}}/\lambda_{\text{val}}^{\text{IPM}}$  in real metals, we would be able to determine the effective electron density  $r_s^{\text{corr}}$  from the equation  $\lambda_{\text{val}}/\lambda_{\text{val}}^{\text{IPM}} = \gamma_{\text{jell}}^{\text{corr}}(r_s^{\text{corr}})$  and read the EMD directly from  $\rho^{2\gamma}(\mathbf{p})$  as  $\rho^e(\mathbf{p}) = \rho^{2\gamma}(\mathbf{p})/\epsilon_{\text{jell}}^{\text{corr}}(p, r_s^{\text{corr}})$  without performing laborious calculations of individual electronic wave functions. The problem of applicability of AED in simple metals is discussed in Ref. 10.

The role of the state selectivity of  $\chi_{\mathbf{k}j}(\mathbf{r})$  is illustrated in Fig. 2, where  $\epsilon_{\text{val}}^{\text{corr}}(\mathbf{p})$ , calculated within the LDA [using  $\epsilon_{\text{jell}}^{\text{corr}}(p, r_s)$  obtained in Ref. 3(h)], presented by a solid line, are compared with enhancement factors following from the state-independent correlation function and from IPM (both denoted by the dashed line).

Let us now focus our attention on momenta  $\mathbf{p}$  outside the FS. For momenta  $|\mathbf{p}|$  greater than the Fermi momentum  $|\mathbf{p}_F|$ ,  $n(\mathbf{p}-\mathbf{G}^*, j^*)=0$ , where  $\mathbf{p}-\mathbf{G}^* \in 1\text{BZ}$ ,  $\mathbf{G}_{\mathbf{k}j^*} = \mathbf{G}^*$  and  $j^*$  is given by relation (13b). In the expression (10) for  $\rho^e(\mathbf{p})$ ,  $n(\mathbf{k}j^*)$  vanishes, and the sum

$$\rho_{\text{NFE}}^e(\mathbf{p}=\mathbf{k}+\mathbf{G}^*) \cong \sum_{j \neq j^*} n(\mathbf{k}j) |u_{\mathbf{k}j}(\mathbf{G}^*)|^2, \quad \mathbf{p} \notin \text{FS}, \quad (17a)$$

where  $\mathbf{G}^* \neq \mathbf{G}_{\mathbf{k}j}$  for  $j \neq j^*$  either vanishes (it happens, e.g., for  $\mathbf{p} \in 1\text{BZ}$  if  $\mathbf{p}_F$  is inside the 1BZ) or is very small [cf. Eq. (13b)]. The amplitudes  $|u_{\mathbf{k}j}(\mathbf{G}^*)|$  for  $j \neq j^*$  are very small as well, and generally no leading term in the

state-independent correlations  $\mathbf{g}(\mathbf{r})$  (Ref. 7) should change visibly the shape of  $\rho_{\text{val}}^{2\gamma}(\mathbf{p})$  with respect to  $\rho_{\text{val}}^e(\mathbf{p})$  and  $\rho_{\text{val}}^{\text{IPM}}(\mathbf{p})$  inside the FS in simple metals. The corresponding parts in experimental curves differ from  $\rho_{\text{val}}^e(\mathbf{p})$  or  $\rho_{\text{val}}^{\text{IPM}}(\mathbf{p})$  only because the two-particle correlations are state selective.

Within LDA the enhancement factor (15b) inside the FS reads as

sum (17a) can be separated. The momentum density is equal to [see Eqs. (14b) and (14c)]

$$\begin{aligned} \rho_{\text{NFE}}(\mathbf{p}=\mathbf{k}+\mathbf{G}^*) &\cong |u_{\mathbf{k}j^*}(\mathbf{G}^*)|^2 |h_{\mathbf{k}j^*}(0)|^2 \\ &\times \sum_{j \neq j^*} |\beta(\mathbf{k}j, \mathbf{G}^*)|^2, \quad \mathbf{p} \notin \text{FS}. \quad (17b) \end{aligned}$$

The resulting enhancement factor is either not determinable [if  $\rho_{\text{NFE}}^e(\mathbf{p})=0$ ] or its momentum dependence is difficult to predict. Even if  $\chi_{\mathbf{k}j}$  are not dependent on the state  $\mathbf{k}j$  (e.g., within IPM), functions  $u_{\mathbf{k}j}(\mathbf{G}^*)$  are [while  $n(\mathbf{k}j)$  switches from unity to zero at  $\mathbf{k}_F$ ], and the momentum dependence of the resulting enhancement factor for momenta  $\mathbf{p}$  outside the FS is observed [in these regions in which  $\epsilon(\mathbf{p})$  is well defined, i.e.,  $\rho^e(\mathbf{p}) \neq 0$ ]. So, for  $\mathbf{p}$  outside the FS it is more convenient to consider  $\rho_j(\mathbf{p})$  and  $\epsilon_j(\mathbf{p})$ , i.e., high momentum components (HMC) of individual bands  $j$ , instead of  $\rho(\mathbf{p})$  and  $\epsilon(\mathbf{p})$ .

## B. High momentum components of annihilation characteristics

We would like to point out that all considerations of this section are general and conclusions should be limited neither to NFE nor to LDA. None of approximations of Sec. IIIA is applied here. This means that our conclusions should be valid also for true correlation functions  $f_{\mathbf{k}j}(\mathbf{r})$ . For real metals these quantities have not been determined by the theory up to now.

The contributions of individual occupied bands  $j$  to  $\rho^e(\mathbf{p})$  and  $\epsilon(\mathbf{p})$  are given by

$$\rho_j^e(\mathbf{k}+\mathbf{G}^*) = n(\mathbf{k}j) |u_{\mathbf{k}j}(\mathbf{G}^*)|^2 \quad (18a)$$

and the corresponding enhancement factor for the occupied state  $\mathbf{k}j$  [cf. Eqs. (12)]

$$\begin{aligned} \epsilon_j(\mathbf{k}+\mathbf{G}^*) &= |h_{\mathbf{k}j}(\mathbf{G}^* - \mathbf{G}_{\mathbf{k}j})|^2 \left| \frac{u_{\mathbf{k}j}(\mathbf{G}_{\mathbf{k}j})}{u_{\mathbf{k}j}(\mathbf{G}^*)} \right|^2 \\ &\times |1 + \alpha(\mathbf{k}j, \mathbf{G}^*)|^2. \quad (18b) \end{aligned}$$

In the band  $j \neq j^*$  (in which the state  $\mathbf{k}j$  is occupied)  $\mathbf{k}+\mathbf{G}_{\mathbf{k}j}$  is responsible for the leading term in  $\rho(\mathbf{p})$  inside the FS, while  $\mathbf{k}+\mathbf{G}^* \neq \mathbf{k}+\mathbf{G}_{\mathbf{k}j}$  provides HMC of these quantities.

In a series of theoretical works<sup>4</sup> devoted to the problem

of electron-positron interactions in the lattice potential, the behavior of HMC in comparison with electrons inside the FS is studied. For this purpose let us define the ratio

$$\begin{aligned} \eta(\mathbf{k}j, \mathbf{G}^*) &= \frac{\varepsilon_j(\mathbf{k} + \mathbf{G}^*)}{\varepsilon_j(\mathbf{k} + \mathbf{G}_{\mathbf{k}j})} \\ &= \left| \frac{h_{\mathbf{k}j}(\mathbf{G}^* - \mathbf{G}_{\mathbf{k}j})}{h_{\mathbf{k}j}(0)} \frac{u_{\mathbf{k}j}(\mathbf{G}_{\mathbf{k}j})}{u_{\mathbf{k}j}(\mathbf{G}^*)} \right|^2 \\ &\quad \times |1 + \delta(\mathbf{k}j, \mathbf{G}^*)|^2, \end{aligned} \quad (19a)$$

where  $\mathbf{G}^* \neq \mathbf{G}_{\mathbf{k}j}$  and

$$\delta(\mathbf{k}j, \mathbf{G}^*) = \frac{\alpha(\mathbf{k}j, \mathbf{G}^*) - \alpha(\mathbf{k}j, \mathbf{G}_{\mathbf{k}j})}{1 + \alpha(\mathbf{k}j, \mathbf{G}_{\mathbf{k}j})}. \quad (19b)$$

The factor  $\eta(\mathbf{k}j, \mathbf{G}^*)$  describes the ratio of enhancements of the HMC and the main component of  $\rho(\mathbf{p})$  inside the FS. Effects  $\eta(\mathbf{k}j, \mathbf{G}^*) > 1$  and  $\eta(\mathbf{k}j, \mathbf{G}^*) < 1$  are usually called overenhancement and de-enhancement, respectively.

The formalism of Ref. 4 leads to the de-enhancement effect only. On the other hand, according to LDA results,<sup>6(d),6(e)</sup> both de-enhancement and overenhancement of HMC are observed in real metals. As follows from Eq. (19), for the chosen vector  $\mathbf{G}^*$  the value of ratio  $\eta(\mathbf{k}j, \mathbf{G}^*)$  depends on (i) the degree of localization of functions  $\chi_{\mathbf{k}j}(\mathbf{r})$  and  $\psi_{\mathbf{k}j}^e(\mathbf{r})$  [i.e., for which the Fourier transforms  $h_{\mathbf{k}j}(\mathbf{G})$  and  $u_{\mathbf{k}j}(\mathbf{G})$  are faster convergent to zero with respect to the reciprocal lattice vectors  $\mathbf{G}$ ]; (ii) the band number, which determines the vectors  $\mathbf{G}_{\mathbf{k}j}$  and  $\mathbf{G}^* - \mathbf{G}_{\mathbf{k}j}$ ; and (iii) the sign of  $\delta(\mathbf{k}j, \mathbf{G}^*)$ , which determines whether the value of the second modulus is greater or smaller than unity.

We would like to stress here that the factor  $\eta(\mathbf{k}j, \mathbf{G}^*)$  depends on the electronic state  $\mathbf{k}j$  even if  $h_{\mathbf{k}j}$  does not (IPM and state-independent correlations<sup>7</sup>), as amplitudes  $u_{\mathbf{k}j}$  depend on  $\mathbf{k}j$ . Also the enhancement factor  $\varepsilon(\mathbf{k} + \mathbf{G}^*)$  appears to be strongly dependent on the momentum in the case of HMC.

The behavior of HMC enhancement factors  $\varepsilon_j(\mathbf{k} + \mathbf{G}^*)$  in Mg is presented in the extended zone scheme in Fig. 3, while the detailed discussion of these results is given in Ref. 10. It should be noted here that our general considerations about over- and de-enhancement of HMC are consistent with results obtained within IPM by Sormann<sup>2(b)</sup> (see also Refs. 10 and 11). Even the fact that neglect of the anisotropy of  $\psi_+$  has only weak influence on the nearest HMC [Ref. 2(b)] is confirmed by our theory.<sup>10</sup>

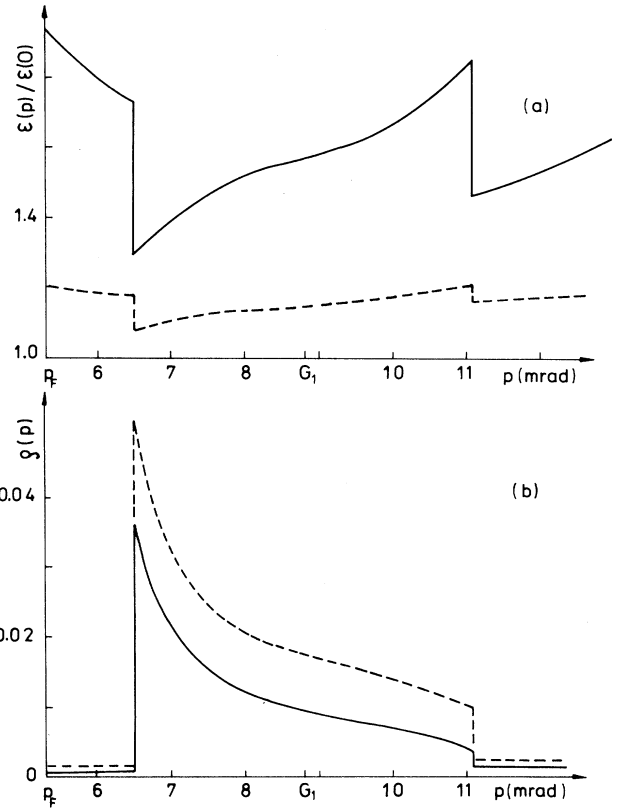


FIG. 3. (a) Enhancement factors  $\varepsilon^{\text{IPM}}(\mathbf{p})$  (solid line) and  $\varepsilon^{\text{corr}}(\mathbf{p})$  (dashed line) along the [100] direction [Ref. 6(e)] in Mg for momenta  $\mathbf{p}$  outside the Fermi surface. For momenta around  $\mathbf{G}_1$  the contribution from the third band dominates in  $\rho(\mathbf{p})$ , i.e.,  $\rho(\mathbf{p}) \cong \rho_3(\mathbf{p})$  and  $\varepsilon(\mathbf{p}) \cong \varepsilon_3(\mathbf{p})$ . Outside this region  $\rho(\mathbf{p}) \cong \rho_1(\mathbf{p})$  and, accordingly,  $\varepsilon(\mathbf{p}) \cong \varepsilon_1(\mathbf{p})$ . (b) The same as in (a) but for  $\rho^\alpha(\mathbf{p})$  and  $\rho^{2\gamma}(\mathbf{p})$  drawn by solid and dashed lines, respectively.

### C. Localized electronic populations

For localized electrons (e.g., those from localized  $d$  bands, in the rare-gas core, at the metal vacancies, or in the near-surface region), in the Fourier representation (9a) of  $\psi_{\mathbf{k}j}^e(r)$  more than one of the amplitudes  $|u_{\mathbf{k}j}(\mathbf{G})|$  are of considerable magnitude, much higher than zero (in contrast to NFE, where only one term was much higher than the other ones). The number of terms  $u_{\mathbf{k}j}(\mathbf{G})$  which should be taken into account in the sum over  $\mathbf{G}$  in the normalization condition (9b), as well as in  $\rho^\alpha(\mathbf{p})$  [Eq. (10)] and  $\rho(\mathbf{p})$  [Eq. (12)], depends on the degree of localization of electronic state  $\mathbf{k}j$ . The sum over  $j \neq j^*$  in (10) and  $\alpha(\mathbf{k}j, \mathbf{G}^*)$  in (12) cannot be neglected, in contrast to the NFE. The resulting enhancement factor

$$\varepsilon(\mathbf{k} + \mathbf{G}^*) = \left[ \sum_j n(\mathbf{k}j) \left| \sum_{\mathbf{H}} u_{\mathbf{k}j}(\mathbf{H}) h_{\mathbf{k}j}(\mathbf{G}^* - \mathbf{H}) \right|^2 \right] / \left[ \sum_j n(\mathbf{k}j) |u_{\mathbf{k}j}(\mathbf{G}^*)|^2 \right] \quad (20)$$

depends on the momentum  $\mathbf{p} = \mathbf{k} + \mathbf{G}^*$  even if  $h_{\mathbf{k}j}$  are state independent, both for  $\mathbf{p}$  inside and outside the FS. For ex-

ample, let us assume that for the occupied state  $\mathbf{k}j^*$  only two terms  $u_{\mathbf{k}j^*}(\mathbf{G}^*)$  and  $u_{\mathbf{k}j^*}(\mathbf{G}^{**})$  ( $\mathbf{G}^{**} \neq \mathbf{G}^*$ ) are not negligible in (9a) [i.e.,  $|u_{\mathbf{k}j^*}(\mathbf{G}^*)|^2 + |u_{\mathbf{k}j^*}(\mathbf{G}^{**})|^2 \cong 1$ ], and the other amplitudes are close to zero. Even if  $h_{\mathbf{k}j}$  is state independent [i.e.,  $h_{\mathbf{k}j}(\mathbf{G}) = h(\mathbf{G})$ ], the corresponding enhancement factor in the band  $j^*$ , equal to

$$\varepsilon_{j^*}(\mathbf{p} = \mathbf{k} + \mathbf{G}^*) \cong |h(\mathbf{0}) + h(\mathbf{G}^* - \mathbf{G}^{**})u_{\mathbf{k}j^*}(\mathbf{G}^{**})/u_{\mathbf{k}j^*}(\mathbf{G}^*)|^2 / |1 + u_{\mathbf{k}j^*}(\mathbf{G}^{**})/u_{\mathbf{k}j^*}(\mathbf{G}^*)|^2,$$

depends on the momentum  $\mathbf{p}$ , as the ratio  $u_{\mathbf{k}j^*}(\mathbf{G}^*)/u_{\mathbf{k}j^*}(\mathbf{G}^{**})$  is momentum dependent.

Thus, for more localized electronic populations the influence of the positron wave function and local state-independent correlations can have a considerable effect on the resulting annihilation characteristics. This fact is confirmed by calculations of  $\rho(\mathbf{p})$  and  $\varepsilon(\mathbf{p})$  performed for core electrons,<sup>8</sup>  $d$  electrons,<sup>7(c)</sup> or at the metal surface.<sup>14</sup>

For strongly varying electron densities (e.g., at the ionic cores or in the near-surface region) the state dependence of  $\chi_{\mathbf{k}j}^{\text{LDA}}(\mathbf{r})$  is much less pronounced than their position dependence and therefore  $\chi_{\mathbf{k}j}(\mathbf{r})$  may be approximated by its average over electronic states  $\mathbf{k}j$ . For less localized electrons ( $d$  electrons), however, neglecting the state dependence of  $\chi_{\mathbf{k}j}(\mathbf{r})$  is not recommended. Features of the enhancement factors for localized electrons are similar to those for HMC: they are strongly momentum dependent and their behavior is difficult to predict.

#### IV. CONCLUSIONS

This paper is devoted to theoretical studies of the momentum dependence of electron-positron enhancement factors for various electron populations in metals. Applications to simple metals are presented in the following paper (Ref. 10).

Our attention has been focused on the influence of the positron distribution and electron-positron correlations on the resulting annihilation characteristics. We have shown on mathematical grounds that for delocalized electronic populations the only effect which visibly changes momentum density  $\rho(\mathbf{p})$  with respect to the EMD within the FS is the state dependence of two-particle electron-positron correlations  $f_{\mathbf{k}j}(\mathbf{r})$ . Neglecting this fact may lead to misleading conclusions about the influence of the positron model on the resulting enhancement factor  $\varepsilon^{\text{corr}}(\mathbf{p})$  in simple metals or to an invalid interpretation of correlation effects in nearly parabolic electronic bands.

In bands of NFE character the AED describes electron-positron correlation effects reasonably well. The main problem is connected with choice of correct electron density<sup>15</sup> when real metal is approximated by model of jellium. The approximation most often applied in theoretical works is the average valence electron density in the Wigner-Seitz cell. This way of determining the effective electron density may be, however, risky even in simple metals, due to the core electron contribution to screening a positron. In the following paper (Ref. 10) we present the effective electron density parameters, describing electron-positron correlations effects in simple metals.

The properties of HMC of  $\varepsilon(\mathbf{p} = \mathbf{k} + \mathbf{G}^*)$  are discussed.

The conditions necessary for observing overenhancement and de-enhancement effects are pointed out. This effect changes both with the band number and reciprocal lattice vector  $\mathbf{G}^*$ . The behavior of HMC depends also on the positron wave function and electron-positron correlations under consideration. Outside the FS  $\varepsilon(\mathbf{p})$  is found to be varying function of momentum, even if IPM or state-independent correlations only are taken into account.

For strongly localized electronic populations dependence of electron-positron correlations on the positron position may be more pronounced than their state dependence. The momentum density  $\rho(\mathbf{p})$  is strongly influenced by the assumed positron distribution in the lattice (cf., e.g., the influence of the correlation potential used in the positron Schrödinger equation on the resulting core enhancement factors<sup>8</sup>). Also the state-independent correlations<sup>7</sup> change appreciably the shape of  $\rho(\mathbf{p})$  inside the FS. Neglecting the state selectivity of two-particle correlations for less-localized electronic bands is, however, not recommended.

#### ACKNOWLEDGMENT

This work is supported by the State Committee for Scientific Research under Grant No. 20 40 49 101.

#### APPENDIX

Within NFE for  $\mathbf{p} \in \text{FS}$  the state  $\mathbf{k}j^*$  is occupied, i.e.,  $n(\mathbf{k} = \mathbf{p} - \mathbf{G}^*, j^*) = 1$ , and  $|u_{\mathbf{k}j}(\mathbf{G}^*)|/|u_{\mathbf{k}j^*}(\mathbf{G}^*)| \ll 1$  for  $j \neq j^*$  [cf. Eqs. (13b) and (13c)], while  $n(\mathbf{k}j) = 0$  or 1, and the number of occupied bands  $j[n(\mathbf{k}j) \neq 0]$  is finite. Thus the sum over  $j \neq j^*$  on the right-hand side of Eq. (10) is small in comparison with  $n(\mathbf{k}j^*) = 1$ , which leads to approximation (14a).

The functions  $\chi_{\mathbf{k}j}(\mathbf{r} = \mathbf{0})$ , i.e., at the ionic core, are equal to zero. This is obvious for the IPM, where  $\chi_{\mathbf{k}j}(\mathbf{r}) = \psi_+(\mathbf{r})$ , as the ionic potential  $V_+(\mathbf{r}) \cong Z/r$  at the center of the atom is strongly repulsive and probability of finding a positron at point  $\mathbf{r} = \mathbf{0}$  is equal to zero. The same result is obtained within the LDA, where

$$\chi_{\mathbf{k}j}(\mathbf{r}) = \psi_+(\mathbf{r}) \{ \varepsilon_{\text{jell}}^{\text{corr}}[\mathbf{k}j, r_s(\mathbf{r})] \}^{1/2},$$

as at the point  $\mathbf{r} = \mathbf{0}$  the electron density is very high [ $r_s(\mathbf{r} = \mathbf{0}) \cong 0$ ] and  $\varepsilon_{\text{jell}}^{\text{corr}}(\mathbf{k}j, 0) = 1$ . Beyond the LDA we have to remember that  $f_{\mathbf{k}j}(\mathbf{r})$ , given by Eq. (6), denote the change of the density of electronic state  $\mathbf{k}j$  on the positron site, assuming that a positron is at point  $\mathbf{r}$ . At the center of the ionic core the electron potential  $V_-(\mathbf{r} \cong \mathbf{0}) \cong -Z/r$  is more attractive than the (un-



screened) electron-positron interaction potential  $V_{ep}(\mathbf{r} \cong \mathbf{0}) \geq -1/r$ . At the extreme case the value of  $f_{kj}(\mathbf{r} = \mathbf{0})$  does not exceed the relative change of electron density at the ionic core when the ionic charge changes

from  $Z$  to  $Z + 1$ . The above density increases at most ten times (cf., e.g., Ref. 16). As a result,  $|\chi_{kj}(\mathbf{r} = \mathbf{0})| = |\psi_+(\mathbf{0})| [f_{kj}(\mathbf{0})]^{1/2} \leq \text{const} |\psi_+(\mathbf{0})| \cong 0$ .

Equation (12a) reads as

$$\rho(\mathbf{k} + \mathbf{G}^*) = |u_{kj^*}(\mathbf{G}^*)|^2 \left[ n(\mathbf{k}j^*) |h_{kj^*}(\mathbf{0})|^2 |1 + \alpha(\mathbf{k}j^*, \mathbf{G}^*)|^2 + \sum_{j \neq j^*} n(\mathbf{k}j) \left| \frac{u_{kj}(\mathbf{G}_{kj})}{u_{kj^*}(\mathbf{G}^*)} \right|^2 |h_{kj}(\mathbf{G}^* - \mathbf{G}_{kj})|^2 |1 + \alpha(\mathbf{k}j, \mathbf{G}^*)|^2 \right]. \quad (\text{A1})$$

Taking into account expansion (11b) and the fact that  $\chi_{kj}(\mathbf{r} = \mathbf{0}) \cong 0$ , we get the relation

$$\chi_{kj}(\mathbf{r} = \mathbf{0}) = \sum_{\mathbf{G}} h_{kj}(\mathbf{G}) \cong 0. \quad (\text{A2})$$

From Eq. (A2) it clearly follows that

$$\sum_{\mathbf{H} \neq \mathbf{G}^*} h_{kj^*}(\mathbf{G}^* - \mathbf{H}) \cong -h_{kj^*}(\mathbf{0}) \quad (\text{A3})$$

and

$$\sum_{\mathbf{H} \neq \mathbf{G}_{kj}} h_{kj}(\mathbf{G}^* - \mathbf{H}) \cong -h_{kj}(\mathbf{G}^* - \mathbf{G}_{kj}). \quad (\text{A4})$$

As a result [Eqs. (A3), (13), and Abel's lemma], the term

$$\left| \sum_{\mathbf{H} \neq \mathbf{G}^*} \frac{u_{kj^*}(\mathbf{H})}{u_{kj^*}(\mathbf{G}^*)} h_{kj^*}(\mathbf{G}^* - \mathbf{H}) \right| \leq \max_{\mathbf{H} \neq \mathbf{G}^*} \frac{|u_{kj^*}(\mathbf{H})|}{|u_{kj^*}(\mathbf{G}^*)|} |h_{kj^*}(\mathbf{0})| \ll |h_{kj^*}(\mathbf{0})|$$

and the value [cf. Eq. (12b)]

$$|\alpha(\mathbf{k}j^*, \mathbf{G}^*)| \ll 1 \quad (\text{A5})$$

can be neglected in the first expression in the square brackets on the right-hand side of Eq. (A1). Similarly [Eqs. (A4), (13), (12b), and Abel's lemma], the expression

$$|\alpha(\mathbf{k}j, \mathbf{G}^*)| \leq \max_{\mathbf{H} \neq \mathbf{G}_{kj}} \frac{|u_{kj}(\mathbf{H})|}{|u_{kj}(\mathbf{G}_{kj})|} \ll 1 \quad (\text{A6})$$

may also be omitted in Eq. (A1). As a result we get the NFE approximation (14b).

<sup>1</sup>For reviews see, e.g., (a) R. N. West, *Positron Studies in Condensed Matter* (Taylor and Francis, London, 1974); (b) P. E. Mijnarends, in *Positron in Solids*, edited by P. Hautojärvi (Springer-Verlag, Berlin, 1979), p. 30; (c) S. Berko, in *Positron Solid State Physics*, edited by W. Brandt and A. Dupasquier (North-Holland, Amsterdam, 1983), p. 102.

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- <sup>9</sup>The experimental papers in which momentum dependence of the enhancement factors in simple metals is studied are cited in Ref. 10, which is the second part of this work.
- <sup>10</sup>G. Kontrym-Sznajd and A. Rubaszek, following paper, Phys. Rev. B **47**, 6960 (1993).
- <sup>11</sup>G. Kontrym-Sznajd, see in *Positron Annihilation* [Ref. 2(c)], p. 691.
- <sup>12</sup>For any lattice vector  $\mathbf{t}$  we have  $\psi_{\mathbf{k}j}^{ep}(\mathbf{r}_e + \mathbf{t}, \mathbf{r}_p + \mathbf{t}) = e^{i\mathbf{k}\mathbf{t}}\psi_{\mathbf{k}j}^{ep}(\mathbf{r}_e, \mathbf{r}_p)$ . This fact follows from the Bloch form (9a) or  $\psi_{\mathbf{k}j}^e(\mathbf{r})$ , the ansatz on the thermalization of the positron (Bloch state 0), and the electron-positron pair momentum conservation principle. As a result, functions  $\chi_{\mathbf{k}j}(\mathbf{r})$  given by Eq. (11a) are periodic in the lattice, i.e.,  $\chi_{\mathbf{k}j}(\mathbf{r} + \mathbf{t}) = \chi_{\mathbf{k}j}(\mathbf{r})$ .
- <sup>13</sup>Lou Yongming, R. M. Nieminen, and B. Johanson, J. Phys.: Condens. Matter **3**, 163 (1991); see in *Positron Annihilation* [Ref. 2(c)], p. 751. Authors of the just-mentioned papers present a "novel" formalism which consists in replacing the electron-positron pair wave function  $\psi_{\mathbf{k}j}^{ep}(\mathbf{r}, \mathbf{r})$  by the product  $\psi_+(\mathbf{r}) \cdot \psi_{\mathbf{k}j}^e(\mathbf{r})$ . This product is considered as the eigenfunction of some one-particle Schrödinger equation. Beyond IPM this procedure is very questionable, e.g., because solutions of the Schrödinger equation require the normalization condition (which is impossible in this case). Moreover, instead of  $\rho^{\text{IPM}}(p)$  or  $\rho^{2\gamma}(p)$  in Al and Si, Yongming *et al.* calculate in practice EMD in these metals. This problem is discussed in detail elsewhere [A. Rubaszek and S. Daniuk (unpublished)].
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