# General properties of electron-positron momentum densities

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We study properties of electron-positron (e-p) momentum densities, especially as concerns the influence on electronic densities of both positron wave-function and correlation effects. General considerations, with a small selection of numerical tests, which prove the validity of our theory, are presented for different models of the positron wave function and for various band-structure calculations. Many-body enhancement and other effects, such as those responsible for the tails in the momentum distribution and the behavior of experimental e-p densities are also discussed.

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## I. INTRODUCTION

In studies of electronic densities in solids, by measuring the angular correlation of annihilation radiation (ACAR) spectra,[1] one gets line or plane integrals of the electron-positron (e-p) momentum density $\rho(\mathbf{p})$ in the extended $\mathbf{p}$ space,

$$\rho(\mathbf{p}) = \sum_{\mathbf{k}j} n_{\mathbf{k}j}\delta(\mathbf{p}-\mathbf{k}-\mathbf{G})\left|\int_{-\infty}^{\infty} e^{-i\mathbf{p}\cdot\mathbf{r}}\psi_{\mathbf{k}j}(\mathbf{r},\mathbf{r})d\mathbf{r}\right|^2. \quad (1)$$

$\psi_{\mathbf{k}j}(\mathbf{r}_e,\mathbf{r}_p)$ is the e-p wave function, $n_{\mathbf{k}j}$ denotes the occupation number of a state $\mathbf{k}$ in the $j$th band, $\mathbf{G}$ is the reciprocal-lattice vector, and $\mathbf{k}$ extends over the first Brillouin zone, the so-called reduced momentum space.

Many-body effects have a considerable influence on observables of positron spectroscopy, first of all on the total annihilation rate, but also on the momentum dependence of the e-p densities. Due to this reason, for a reliable interpretation of experimental positron annihilation data, an understanding of these effects is of vital importance. An ideal theoretical description of the e-p annihilation in metals should include both e-p and electron-electron (e-e) correlations (positron-positron interaction can be neglected, due to the small number of these particles in the crystal). Taking into account the complexity of such a many-body problem, it is evident that it can be solved only within severe approximations. All theoretical approaches (except for Arponen and Pajanne's theory[2]) are based on the following result of Carbotte and Kahana:[3] An annihilating e-p pair, seen from outside, behaves like a neutral quantity, so no tail beyond the Fermi momentum should be observed in the e-p momentum density.

For a long time, this result had been considered almost an axiom. Meanwhile, new two-dimensional (2D) ACAR experiments[4–8] clearly demonstrate that the observed smearing of the Fermi surface (FS) and considerable high-momentum tails are due to e-e correlations playing a significant role above the FS. For example, Manuel *et al.*,[5] studying the FS smearing in experimental 2D ACAR spectra for Al, performed an analysis with very precisely determined experimental resolution functions. They found a presence of tails above the Fermi momentum $p_F$ and interpreted it as an effect of e-e correlations. Such effects are evidently visible in Compton experiments, e.g., Ref. 9 and references therein. They may be theoretically described (in the simplest approximation) by the isotropic Lam-Platzman correction,[10] or, more effectively, by $GW$ calculations.[11–13] Such correlations influence the electron momentum density by reducing the momentum step at the FS and by the appearance of a momentum tail above $p_F$. As a consequence, the anisotropy of the profiles is also decreased.

In the case of metallic crystals where electrons and positrons move within a lattice potential, an ideal theory should also include the influence of such a potential on correlation effects. An attempt in this direction is the Bloch-modified ladder (BML) theory[14] (based on earlier papers[15,16]) where this is taken into account by calculating both interband and intraband transitions of the annihilating Bloch particles. However, this theory has several shortcomings: It requires a large amount of computer effort, and it includes some approximations causing strong deenhancement effects within the high-momentum region, up to now not confirmed by the experiment. Due to these reasons, most calculations of e-p momentum densities are based on electron and positron wave functions, received from band-structure calculations within the independent particle model (IPM), multiplied by enhancement factors obtained by many-body theories for the positron in a homogeneous electron gas.

Recently, Laverock *et al.*,[17] proposed introducing model functions including empirical enhancement factors. In opposition to other authors, they studied correlation effects (attributed to e-p correlations) by interpreting 2D ACAR spectra folded into the reduced $\mathbf{k}$ space.[18,19] From the point of view of FS studies, working within the reduced $\mathbf{k}$ space is very useful because one expects that FS steps should be better marked. However, what could be the physical meaning of correlation effects determined in the $\mathbf{k}$ space?

Sections II–IV of the present paper are dedicated to all these topics. First of all, we want to answer the question concerning the physical meaning of empirical correlation factors determined in the $\mathbf{k}$ space if the corresponding e-p correlation functions—defined via e-p wave functions—are determined in the extended $\mathbf{p}$ space. In our point of view, such a conversion of the correlation factor from the $\mathbf{p}$ into the $\mathbf{k}$ zone is acceptable if the correlation effects are dependent on $\mathbf{k}$ but not on the reciprocal-lattice vector $\mathbf{G}$. However, as shown in the present paper, enhancement factors, due to many-body effects, do significantly depend on $\mathbf{G}$. This is shown in Sec. II where we present a small selection of test results performed

 

for alkalis, Al, Cu, and Pd and for two various approaches of the e-p interaction, used for the calculation of enhancement factors for two valence electron bands in Cu.

A further question, studied in Sec. III, deals with the main conclusion of Carbotte and Kahana's theory[3] on positrons in a homogeneous electron gas, namely, that there is no tail of the e-p momentum density beyond the Fermi momentum. The question is if this conclusion is correct, and if yes, whether it is also valid for real metals.

Of course, for a reliable comparison of experimental results with various theoretical calculations, it must be guaranteed that all differences observed are caused by different models of the e-p correlations and not by uncertainties due to approximations of electron and positron wave functions or to various band-structure methods. Therefore, in Sec. IV, we check the sensitivity of e-p momentum densities within the IPM, using various approximations in the calculating of both electron and positron wave functions. Numerical tests are based (i) on augmented plane-wave (APW) calculations and three different models of the positron wave function,[20–22] and (ii) on the full-potential linear APW (FP-LAPW) program WIEN2K[23] with using three different crystal potentials (more details in Sec. IV). It should be noticed here that all these models were also used in our tests presented in Sec. II, just to confirm that conclusions in Sec. II were general, independent of both models of the positron wave function and various band-structure methods.

In Sec. V, we show a diversity in behavior of experimental e-p momentum densities in order to illustrate difficulties in describing them within theories which ignore the influence of the lattice potential on the e-p interaction.

## II. ELECTRON-POSITRON MOMENTUM DENSITIES

In a periodic lattice potential, the e-p density in the $j$th band can be written, within the IPM, as[24]

$$\rho_j^{\mathrm{IPM}}(\mathbf{k}+\mathbf{G}) = n(\mathbf{k}j)|u_{\mathbf{k}j}(\mathbf{G}_{\mathbf{k}j})|^2|v(\mathbf{G}-\mathbf{G}_{\mathbf{k}j})|^2[1+\alpha_{\mathbf{k}j}(\mathbf{G})]^2, \quad (2)$$

where

$$\alpha_{\mathbf{k}j}(\mathbf{G}) = \sum_{\mathbf{H}\neq\mathbf{G}_{\mathbf{k}j}} \frac{v(\mathbf{G}-\mathbf{H})u_{\mathbf{k}j}(\mathbf{H})}{v(\mathbf{G}-\mathbf{G}_{\mathbf{k}j})u_{\mathbf{k}j}(\mathbf{G}_{\mathbf{k}j})}. \quad (3)$$

$u_{\mathbf{k}j}$ and $v$ are Fourier coefficients of the wave functions of the electron and the thermalized positron, respectively. $\mathbf{H}$ and $\mathbf{G}_{\mathbf{k}j}$ are reciprocal-lattice vectors, where $\mathbf{G}_{\mathbf{k}j}$ corresponds to the *leading* Fourier coefficient of the electron wave function with the property $|u_{\mathbf{k}j}(\mathbf{G}_{\mathbf{k}j})| > |u_{\mathbf{k}j}(\mathbf{H})|$, whereas, the $u_{\mathbf{k}j}(\mathbf{H})$'s belong to the Umklapp components. Such a description of a two-particle density and knowledge of general properties of the parameters $\alpha$ allow for determining some general rules connected with features of $\rho(\mathbf{p})$.[24,25]

An influence of the positron wave function on the electron density $\rho^e$ and the effects of e-p correlations, respectively, are studied through the following enhancement factors:

$$\varepsilon^{\mathrm{IPM}}(\mathbf{k}+\mathbf{G}) = \rho^{\mathrm{IPM}}(\mathbf{k}+\mathbf{G})/\rho^e(\mathbf{k}+\mathbf{G})$$

and $$\varepsilon^{\mathrm{corr}}(\mathbf{k}+\mathbf{G}) = \rho(\mathbf{k}+\mathbf{G})/\rho^{\mathrm{IPM}}(\mathbf{k}+\mathbf{G}).$$

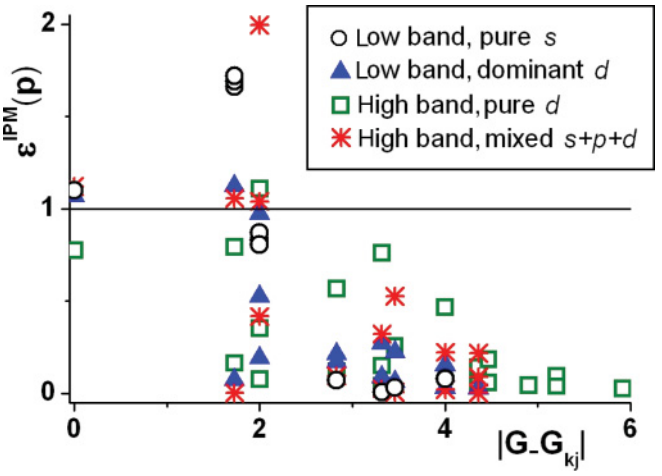


FIG. 1. (Color online) $\varepsilon_j^{\mathrm{IPM}}(\mathbf{p})$ for different electron states in Cu as a function of $|\mathbf{G}-\mathbf{G}_{\mathbf{k}j}|$ (in units of $2\pi/a$ with the lattice constant $a = 6.8308$ a.u.). All values for $|\mathbf{G}-\mathbf{G}_{\mathbf{k}j}| = 0$ belong to the leading momentum component, and $|\mathbf{G}-\mathbf{G}_{\mathbf{k}j}| \neq 0$ for Umklapp components.

For the leading terms of the density [insert $\mathbf{G} = \mathbf{G}_{\mathbf{k}j}$ into Eq. (2)], $\varepsilon_j^{\mathrm{IPM}}(\mathbf{k}+\mathbf{G}_{\mathbf{k}j})$is simply given by

$$\varepsilon_j^{\mathrm{IPM}}(\mathbf{k}+\mathbf{G}_{\mathbf{k}j}) = |v(\mathbf{0})|^2[1+\alpha_{\mathbf{k}j}(\mathbf{G}_{\mathbf{k}j})]^2. \quad (4)$$

According to our theoretical predictions,[24,25] absolute values of the parameter $\alpha(\mathbf{G}_{\mathbf{k}j})$ are considerably smaller than 1, and negative $\alpha(\mathbf{G}_{\mathbf{k}j})$ are expected for pure $d$ states. This is confirmed by our numerical calculations: For alkalis, the lowest and highest values of $\alpha$ correspond to Li (0.038) and Cs (0.125), respectively, and among the transition metals Cu and Pd, the highest values of $\alpha$ are observed for Pd (0.172 for *spd* states). Only for pure $d$ states, did we obtain negative values of $\alpha$ ($-0.061$ for Pd and $-0.088$ for Cu).

Since $|v(\mathbf{0})| < 1$, which follows from the norm of the positron wave function, negative coefficients $\alpha_{\mathbf{k}j}(\mathbf{G}_{\mathbf{k}j})$ always lead to a reduction in the corresponding main density $d$-state components. Other states could be intensified if $\alpha_{\mathbf{k}j}(\mathbf{G}_{\mathbf{k}j}) > 1/|v(\mathbf{0})| - 1$ where this condition is only valid for positive $\alpha_{\mathbf{k}j}(\mathbf{G}_{\mathbf{k}j})$'s and for states $\mathbf{k}j$ for which lattice effects are high. Such conclusions are confirmed by our numerical tests: Among 16 cases, which we studied, $\varepsilon_j^{\mathrm{IPM}}(\mathbf{k}+\mathbf{G}_{\mathbf{k}j})$ is greater than 1 in 14 cases, changing from 1.03 (Al) to 1.25 (Pd, *spd* states) and less than 1 only for pure $d$ bands (0.78 in Cu and 0.80 in Pd).

Similar considerations for Umklapp components (for more details, see Refs. 2 and 3) lead to the conclusion that $\varepsilon_j^{\mathrm{IPM}}(\mathbf{k}+\mathbf{G})$, state dependent through $\alpha_{\mathbf{k}j}(\mathbf{G})$, is strongly dependent on the reciprocal lattice vector $\mathbf{G}$. In comparison to $\rho^e(\mathbf{k}+\mathbf{G})$, the intensities of the Umklapp components of $\rho^{\mathrm{IPM}}(\mathbf{k}+\mathbf{G})$ are generally reduced, with the exception of some of the first components, which may be intensified. All this is confirmed by our numerical results where a small selection of them is displayed in Fig. 1 and in the $\varepsilon^{\mathrm{IPM}}$ curves of Fig. 3.

As a consequence of such a strong dependence of the density $\rho^{\mathrm{IPM}}(\mathbf{p} = \mathbf{k}+\mathbf{G})$ on the reciprocal-lattice vector $\mathbf{G}$, the Lock-Crisp-West-folded density $\rho^{\mathrm{IPM}}(\mathbf{k})$ will be strongly dependent on $\mathbf{k}$. For this reason, the e-p densities $\rho(\mathbf{k})$ do not

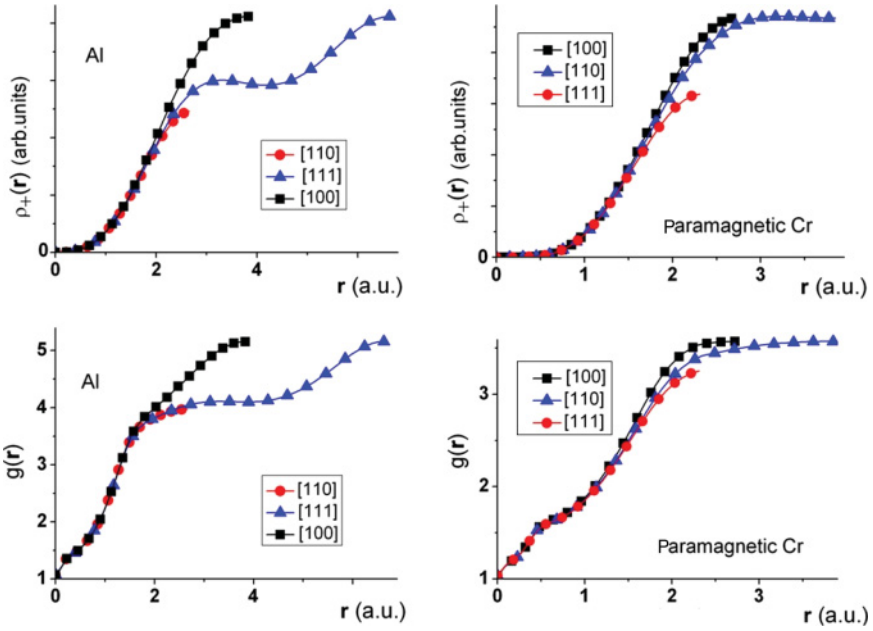


FIG. 2. (Color online) Positron density $\rho_+(\mathbf{r})$ and e-p correlation function $g(\mathbf{r})$ in fcc Al and paramagnetic bcc Cr along three main symmetry directions in the unit cell. All functions are drawn from $r = 0$ (position of the atom) up to their maximum value in the interstitial region.

resemble the steplike function as they do in the case of electron densities.

When studying e-p correlation effects where the e-p wave function can approximately be written in the form $\psi^{e-p}_{\mathbf{k}j}(\mathbf{r},\mathbf{r}) = \psi_{\mathbf{k}j}(\mathbf{r})\tilde{\psi}^{+}_{\mathbf{k}j}(\mathbf{r})$, the positron wave function, renormalized with respect to many-body effects by $f_{\mathbf{k}j}$, can be defined as

$$\tilde{\psi}^{+}_{\mathbf{k}j}(\mathbf{r}) = f_{\mathbf{k}j}(\mathbf{r})\psi_{+}(\mathbf{r}), \tag{5}$$

where $\psi^{+}(\mathbf{r})$is the IPM positron wave function.

Both functions $f_{\mathbf{k}j}(\mathbf{r})$ and $\tilde{\psi}^{+}_{\mathbf{k}j}(\mathbf{r})$, where $\mathbf{r}$ denotes the position of both the electron and the positron, are periodic in the lattice, i.e., they can be expanded into Fourier series with respect to the reciprocal-lattice vectors. Thus, Eq. (2) can be rewritten for e-p densities where the coefficients $v$ are replaced by the Fourier coefficients of the renormalized positron wave functions. The main difference between $\tilde{\psi}^{+}_{\mathbf{k}j}(\mathbf{r})$ and $\psi^{+}(\mathbf{r})$ comes from the fact that $\tilde{\psi}^{+}_{\mathbf{k}j}(\mathbf{r})$ is not normalized to unity and is strongly state dependent via correlation effects.

The e-p correlations could be expressed within the local density approximation (LDA) via the contact value of the e-p correlation function $g[\mathbf{r}_e - \mathbf{r}_p;\ r_s(\mathbf{r}_p)] \equiv g(\mathbf{r}_p)$. We will further call that quantity correlation function $g(\mathbf{r})$, and $r_s \equiv r_s(\mathbf{r})$ is the local electron-density parameter (radius of the sphere containing one electron). In the case of a state-independent approximation, it is simply given by

$$\tilde{\psi}^{+}(\mathbf{r}) = \sqrt{g(\mathbf{r})}\psi_{+}(\mathbf{r}).$$

In this paper, for $g(\mathbf{r})$, we use the well-known formula by Boronski-Nieminen[26] (B-N),

$$g(\mathbf{r}) = 1 + 1.23r_s + 0.8295r_s^{3/2} - 1.26r_s^2 + 0.3286r_s^{5/2} + r_s^3/6. \tag{6}$$

This function describes quite well the experimental positron lifetime $\tau$ ($\tau = 1/\lambda$, where $\lambda$ denotes the total annihilation rates) in metals—i.e., it can be treated as a real enhancement factor, averaged over the electron states $\mathbf{k}j$. A comparison of $\mathbf{r}$ dependencies of the B-N correlation function $g(\mathbf{r})$ and the positron density $\rho_+(\mathbf{r})$ within the unit cells of the simple metal Al and the transition metal (paramagnetic) Cr is presented in Fig. 2. As seen, $g(\mathbf{r})$ has a similar shape to $\rho_+(\mathbf{r})$, being positive and increasing with $\mathbf{r}$, with a tendency to saturate in the interstitial region [such a behavior can also be observed for the local density parameter $r_s(\mathbf{r})$ and for $f_{\mathbf{k}j}(\mathbf{r})$]. This follows from the fact that the electron density $\rho(\mathbf{r})$ decreases with $\mathbf{r}$ while the e-p correlation function decreases with increasing $\rho(\mathbf{r})$. This leads to quite different values of $g(\mathbf{r})$ for Al and Cr as seen in Fig. 2 and to large values for, e.g., potassium where the correlation function even approaches 20.

This similarity of the dependencies of $g(\mathbf{r})$ and $\rho_+(\mathbf{r})$ on $\mathbf{r}$ allows us to draw similar conclusions as obtained before for $\varepsilon^{\mathrm{IPM}}$:

(1) in the momentum space, the higher-momentum components of electronic densities are mostly reduced via the e-p interaction potential;

(2) even a state-independent correlation function will enhance a dependence of $\varepsilon^{\mathrm{corr}}(\mathbf{k}+\mathbf{G})$ on both the state $\boldsymbol{k}j$ and the reciprocal-lattice vector $\mathbf{G}$, similarly as in the case of $\varepsilon^{\mathrm{IPM}}_j(\mathbf{k}+\mathbf{G}_{\mathbf{k}j})$.

As a prominent example of a state- and energy-dependent approximation of the correlation function, leading to

$$\tilde{\psi}^{+}_{\mathbf{k}j}(\mathbf{r}) = \sqrt{g(\mathbf{r},\mathbf{k}j)}\psi_{+}(\mathbf{r}),$$

we used the LDA formula as proposed in Ref. 27.

Apart from the presented B-N and LDA($E$) approach, the literature also offers some more realistic approaches for the correlation function $f_{\mathbf{k}j}(\mathbf{r})$, which are, however, much more complicated: Beyond some effects of nonlocality,[28,29] the correlation effects are influenced by the lattice potential[14–16] as, e.g., within the BML theory, also applied in this paper.

In Fig. 3, using the example of Cu (it combines features of simple and transition metals), we demonstrate how similarity of the dependencies of $g(\mathbf{r})$ and $\rho_+(\mathbf{r})$ on $\mathbf{r}$ reveals the corresponding enhancement factors in the momentum space. It is clear that it introduces a strong dependence of the enhancement on the reciprocal vector—this is characteristic

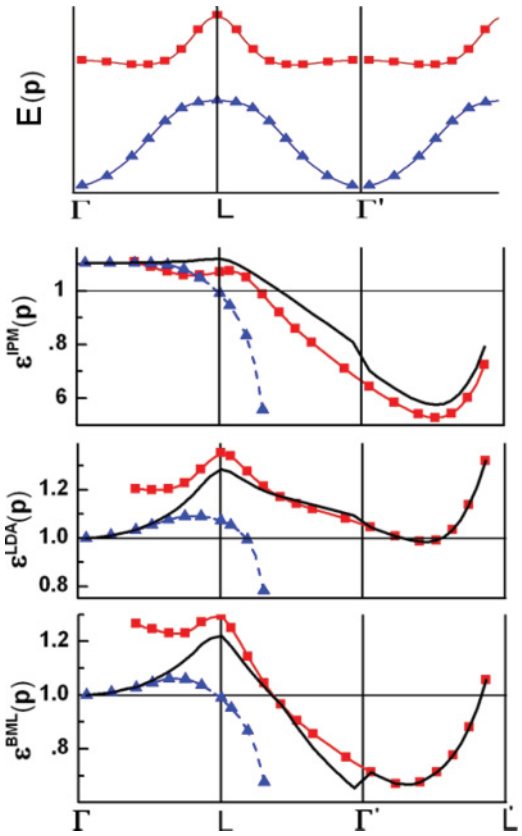


FIG. 3. (Color online) Two electron bands in Cu along the [111] direction, which contribute to e-p momentum densities and corresponding enhancement factors calculated within LDA($E$) and BML theory. The full line shows the enhancement factor for the total densities.

of all models. Additionally, in the case of Cu, both theories [LDA($E$) and BML] give the typical monotonic increase in the Kahana-like enhancement[30] with increasing momentum $\mathbf{p}$ inside the FS. For momenta above FS, there is a strong deenhancement of the Umklapp components in the case of BML theory (the reduction in the Umklapp components in favor of the main component is a tendency of this theory).

Another theoretical approach[31,32] is based on a state-dependent correlation factor $f_{\mathbf{k}j}(\mathbf{r}) = g_{\mathbf{k}j}$, independent of $\mathbf{r}$, which leads to the momentum dependence of the enhancement factor $\varepsilon(\boldsymbol{p})$ similar to B-N theory. The more recent weighted density approximation[28,29] uses both nonlocal and energy-dependent e-p correlation functions. The resulting momentum dependence of the enhancement is similar to LDA($E$) for simple metals while, for transition metals, is somewhat reduced (but still much higher than in BML theory). As far as all approaches, mentioned in this section, differ in many aspects, they have a common feature: They describe only static e-p correlations, i.e., they ignore dynamical correlations described in the next section.

## III. SELF-ENERGY EFFECTS

As Carbotte and Kahana claimed,[3] the e-p momentum distribution characterized by a high-momentum tail could not be seen by the positron because the dynamic parts of the e-p interaction would reduce the influence of the electron as well as the positron on the other electrons. In order to have deeper insight into the problem, let us, at first, look at some details of the approach.[3] Due to its interaction, the electron polarizes the electronic medium, and the arising net charge dynamically influences the electron itself. Therefore, the probability of spending some time above the FS is greater than zero, the tails arise above the FS, and the occupation numbers below the FS become less than 1. Since the energy of the given electron is changed during the process of self-interaction with the medium, the phenomenon is commonly called the self-energy effect.

To the first order, the change in momentum distribution $\rho(\mathbf{p})$, due to the above effect, can be described with Green's-function formalism in the following way:[3]

$$\rho^{\text{e.s.e.}}(p) = i\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\frac{i}{\Omega}\sum_{\mathbf{k}}\int_{-\infty}^{\infty}\frac{d\omega'}{2\pi}u(\mathbf{k};\omega') \times\left[G_e^0(\mathbf{p};\omega)\right]^2 G_e^0(\mathbf{p}-\mathbf{k};\omega-\omega'), \quad (7)$$

where

$$G_e^0(\mathbf{p};\omega) = \frac{\theta(p_F-|\mathbf{p}|)}{\hbar^2p^2/2m_e-\omega+i0^+} + \frac{\theta(|\mathbf{p}|-p_F)}{\hbar^2p^2/2m_e-\omega-i0^+} \quad (8)$$

is a free particle propagator and $u(\mathbf{k};\omega)$ is the dynamic random-phase approximation (RPA) potential in which the polarization is described by the frequency-dependent Lindhard function. According to the notation of Ref. 3, the labels e.s.e., p.s.e., and h.d. mean electron self-energy, positron self-energy, and high density, respectively.

If there were no e-p interactions, the quantity $\rho(p) = \rho^{\text{e.s.e.}}(p)$ could be described with the Daniel-Vosko curve (Fig. 2 in Ref. 33). However, similar to the electron case, positron self-energy effects appear when the positron interacts with the electronic medium. The corresponding polarization makes the positron momentum distribution different from Dirac's $\delta$ peak, smearing it out around $p = 0$.

It turns out that the positron self-energy contribution $\rho^{\text{p.s.e.}}$ can also be described by Eq. (7), provided that $G_e^0(\mathbf{p},\omega)$ is replaced by the positron Green's function $G_p^0(\mathbf{p},\omega)$, the electron mass is replaced by the positron one, and $p_F = 0$. Then, the quantity $\rho^{\text{p.s.e.}}$ is of the same sign and order of magnitude as $\rho^{\text{p.s.e.}}$ and adds to the electronic effect.[3] Both effects just smooth out the momentum distribution (however, the jump at $k_F$ still remains) and produce quite considerable tails above the FS. If the e-p interaction is, however, switched on, the situation changes dramatically, at least, for the electron gas and the contribution (9) to $\rho(p)$,

$$\rho^{\text{h.d.}}(p) = \frac{i}{\Omega}\sum_{\mathbf{kq}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{d\omega\,d\omega' d\omega''}{(2\pi)^3}u(\mathbf{k};\omega') \times G_e^0(\mathbf{k}+\mathbf{q};\omega+\omega')G_e^0(\mathbf{q};\omega') \times G_p^0(\mathbf{p}-\mathbf{q}-\mathbf{k};\omega''-\omega)G_p^0(\mathbf{p}-\mathbf{q};\omega'') \quad (9)$$

has the opposite sign to self-energy terms and effectively cancels the e-p momentum distributions above $p_F$. Then,

$$\rho(p > p_F) = \rho^{\text{e.s.e.}}(p) + \rho^{\text{p.s.e.}}(p) + \rho^{\text{h.d.}}(p) \cong 0. \quad (10)$$

In fact, the suppressed tail has also been found in recent Monte Carlo calculations.[34] Although slightly bigger than those in Refs. 3 and 34, small tails appeared in the very sophisticated bosonic approach of Arponen and Pajanne.[2]

So far, we discussed the problem of many-body tails when calculated only for the first order in perturbation theory. Carbotte and Kahana estimated, however, that the cancellation of the tail still would occur in all orders of perturbation. They showed that the enhancement effects connected with increased electron density around the positron could, in principle, work as if the first-order quantities of $\rho(p)$ for $p > p_F$ were multiplied by some value of the enhancement at $p_F$. The only many-body momentum-dependent enhancement factors for the electron gas (if not counting BML theory for crystals[14]), known almost to date have been determined for $p < p_F$. The attempt to calculate the enhancement factors for all values of momenta has recently been undertaken by Boroński,[35,36] who solved a modified Bethe-Goldstone equation, including approximately, in all orders, electron self-energy effects. Of course, if the cancellation discussed above always occurs, these factors would not have any substantial meaning, otherwise, one should take them into account.

One should underline that the calculation of all effects leading to the cancellation of the momentum tail have been performed for the "one-positron-many-electrons" system within a spatially homogeneous electron gas. In this environment, the Carbotte-Kahana canceling of the e-p momentum tails beyond $p_F$ may be valid in good approximation. However, there is no certainty that this result will also be true for a positron within the inhomogeneous electron gas in a crystal. Since a more precise answer would require tedious band-structure and spectral function calculations, not always fully feasible, for now, one proposes an estimation of this effect within a simple model[37] where one assumes the effective-mass approach for the calculation of electron and positron self-energies with the dynamic effective potential in the RPA approximation. In this instant, one can utilize all the formulas presented above to calculate $\rho(\mathbf{p})$ but with free electron and positron masses $(m_e,m_p)$ appropriately replaced in formulas (7)–(9) by the electron and positron effective masses $(m_e^*,m_p^*)$. Then,

$$\rho(p > p_F) = m_e^*\rho^{\text{e.s.e.}}(m_e^*; p) + m_p^*\rho^{\text{p.s.e.}}(m_e^*,m_p^*; p) + \rho^{\text{h.d.}}(m_e^*,m_p^*; p), \quad (11)$$

where the dependence in $\rho^{\text{p.s.e.}}$ on $m_e^*$ appears because of introducing $m_e^*$ into the effective interaction $u(\mathbf{k};\omega)$. As an example, we have performed calculations for $m_e^* = 2$ and, to make a comparison with Table I of Ref. 3, the electron density (defined in Ref. 3 via $\alpha$) corresponds to $r_s = 3.79$ $(\alpha = 0.2)$.

In comparison to Carbotte and Kahana's calculations where $m_e^* = m_p^* = 1$, for $m_e^* = 2$ and $m_p^* = 1$, the reduction in the tail is much weaker (see Fig. 4), and the momentum distribution "seen" by the positron is half the distribution of Daniel and Vosko.[33] This effect could be even slightly enlarged, and the overall (for $p < p_F$ and for $p > p_F$) many-body enhancement may be less visible in angular correlation curves if the enhancement factor was calculated according to Ref. 36 where electron self-energy effects are incorporated in calculations of Bethe-Goldstone amplitude. Thus, the dynamic e-p interaction

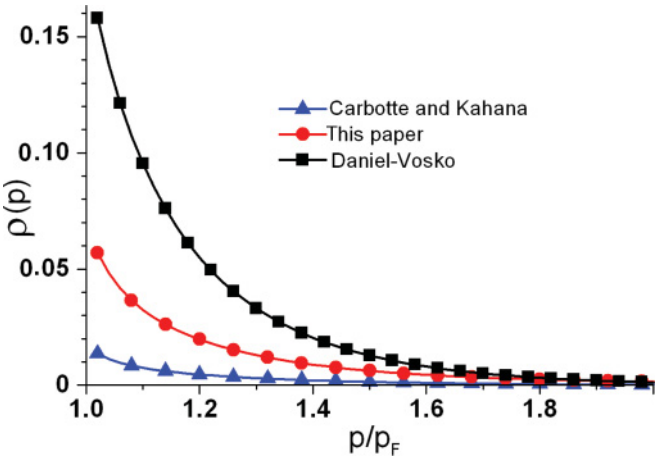


FIG. 4. (Color online) High-momentum tail in $\rho(p)$. The curve with triangles corresponds to values from Table 1 of Ref. 3 when the considerable cancellation of somecontributions occurs. The line with the balls corresponds to our calculations for $m_e^* = 2$ and $m_p^* = 1$. The curve with the squares corresponds to the case when only e-e correlations are taken into account (Ref. 33).

cannot sufficiently reduce the momentum tail to make it negligible. More so, if the effective mass of the electron increases, the tail becomes even more substantial[37] since the electron self-energy contribution grows up faster than the other terms. The same rules would diminish the $\rho(\mathbf{p})$ values below $p_F$, making the whole distribution far different from the rectangular one.

The presented estimation is, of course, simplified, but it clearly shows how much many-body tails in momentum distributions may depend on details of the electronic structure of a given element.

## IV. SENSITIVITY OF $\rho^{\text{IPM}}(p)$ TO VARIOUS APPROXIMATIONS OF THE ELECTRON AND POSITRON WAVE FUNCTIONS

When comparing theory with experimental results, one must be sure that all differences observed are connected with various models for many-body effects, not to uncertainties due to approximations of e-p wave functions or to various band-structure methods—this is the topic of this section.

It is well known that many of the Fourier coefficients of $\psi_+(\mathbf{r})$ are remarkably sensitive to approximations of both various potentials and the positron wave function.[38,39] Nevertheless, according to a finding for the alkalis, Cu, and Pd,[38] the high-momentum components of the e-p density close to the central Brillouin zone—or, in the case when the FS extends over more than one band, close to the Brillouin zone containing the leading term of density—are not very sensitive to details in the shape of $\psi_+(\mathbf{r})$. A similar effect for total annihilation rates has been observed by the authors of Ref. 40. A theoretical explanation of these effects, based on general considerations, has been given in Ref. 41: In each metal, there are some components of $\rho^{\text{IPM}}(\mathbf{p})$, which are largely independent of uncertainties arising from different approximations of $\psi_+(\mathbf{r})$. Moreover, such *stable* densities mainly correspond to densities of high values (leading term

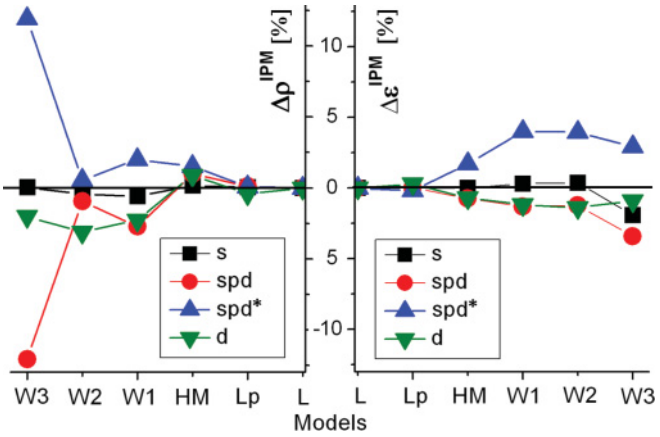


FIG. 5. (Color online) Relative changes in $\Delta\rho^{\mathrm{IPM}}$ and $\Delta\varepsilon^{\mathrm{IPM}}$ [in percentages of their values for the L model] for the leading terms of density in Pd for: pure $s$, pure $d$, dominant $d$ ($spd^*$), and mixed $s+p+d$ ($spd$) electron states.

of the density and the highest Umklapp components), which can easily be studied in the experiment. This statement is strongly supported by our numerical tests (Figs. 5–7) based on APW calculations where the notations L, Lp, and HM refer to different models of the positron wave function: L means the muffin-tin approximation proposed by Loucks,[20] Lp corresponds to a *perturbed* Loucks positron wave function,[21] and HM is a more realistic description of $\psi_+(\mathbf{r})$ as established by Hubbard and Mijnarends.[22] Second, in order to check how $\rho^{\mathrm{IPM}}(\mathbf{p})$ reacts to changes in both the electron and the positron wave functions obtained by quite different band-structure methods as well as by different crystal potentials, we also used the FP-LAPW program WIEN2K (Ref. 23), including the following potentials: W1—nonrelativistic LDA; W2—nonrelativistic generalized gradient approximation (GGA); W3—scalar-relativistic GGA. Results concerning the leading terms of densities of various electronic states in Pd are presented in Fig. 5 where it is shown that the sensitivity of these terms, with respect to changes in the positron wave function (compare results for L, Lp, and HM), is very small—less than 2% for all examples investigated. When both electron and positron wave-function calculations are performed using essentially different band-structure methods (e.g., the FP-LAPW instead of the APW), the $\Delta\rho^{\mathrm{IPM}}$ values may be somewhat higher. However, when scalar-relativistic potential (W3) is used, differences become much greater, in particular, in metals, as, e.g., in Pd where relativistic effects play a significant role. Fortunately, corresponding changes in the enhancement factor $\varepsilon$ are not so large (in the case of Pd and used models $\Delta\varepsilon < 4\%$) because $\varepsilon$ is the ratio of two densities (without and with correlations), which have been calculated within the same formalism.

In Figs. 6 and 7, we present results for Umklapp components of various electronic states of Al and Pd, respectively, depending on their distance from the leading term of the density, given by $\mathbf{G}_i$ where index $i=0$ means the leading term and $i=1$, $1'$ or $1''$ denotes various reciprocal-lattice vectors with the lowest (i.e., first) distance from the leading terms, $i=2$, $2'$, or $2''$—second distance, etc.

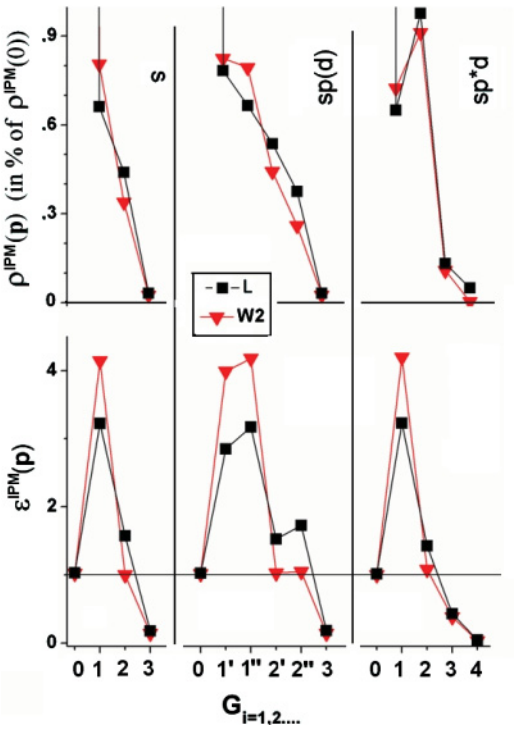


FIG. 6. (Color online) $\rho^{\mathrm{IPM}}(\mathbf{k}+\mathbf{G})$ and $\varepsilon^{\mathrm{IPM}}(\mathbf{k}+\mathbf{G})$ in Al vs the reciprocal-lattice vector $\mathbf{G}$ for various electron states and two models (L and W2) of electron and positron wave functions. $sp(d)$ means $s+p$ with a small $d$ contribution, and $sp^*d$ means $p$ dominant $s+p+d$ mixture.

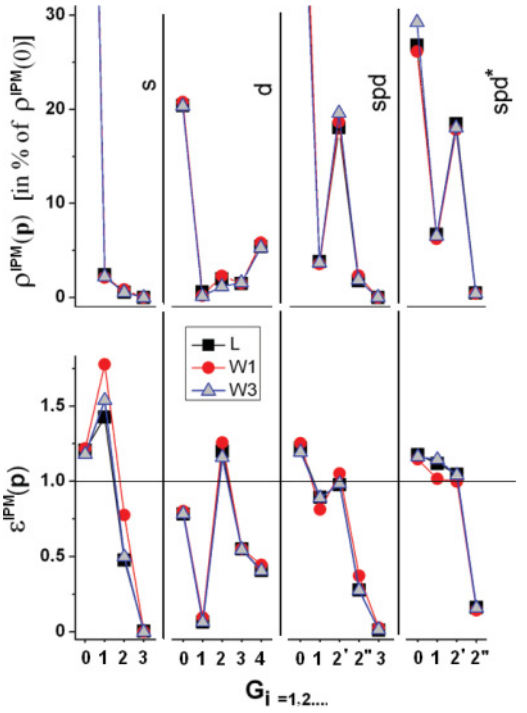


FIG. 7. (Color online) The same as in Fig. 6 but for Pd and three models (L, W2, and W3) of electron and positron wave functions.

In the case of Al, relativistic effects are negligible, so we restrict our investigations to the L and W2 "models." Taking into account that maximal values of Umklapp components are lower than 1% of $\rho^{\mathrm{IPM}}(\mathbf{p} = \mathbf{0})$, differences between densities for these two models can be neglected in relation to the experimental accuracy. Compared to that, one observes rather large changes concerning the absolute values of the enhancement factors $\varepsilon^{\mathrm{IPM}}(\mathbf{p})$. However, we should take into account that, in ACAR experiments, one studies only the relative values of densities. Therefore, we are more interested in the momentum dependence [i.e., the shape of $\varepsilon^{\mathrm{IPM}}(\mathbf{p})$], which is almost the same for both models L and W2. Of course, a problem could arise if we would like to consider such subtle effects as, e.g., overenhancement of the second Umklapp components. However, this refers to very small densities [lower than 1% of $\rho^{\mathrm{IPM}}(\mathbf{p} = \mathbf{0})$], too small for experimental investigations.

The results for Pd, displayed in Fig. 7, differ significantly from those for Al: the Umklapp components in Pd are essentially larger what is typical for transition metals. Taking into account that the two models L and W3 are substantially different, the disagreement of the corresponding results—especially as it concerns the Umklapp components—is surprisingly small.

So, one could expect that theoretically obtained values of $\rho^{\mathrm{IPM}}(\mathbf{p})$ (provided, of course, that a powerful band-structure code is used) can be used as a quality test of different theoretical descriptions of many-body effects, provided the following limits are taken into account:

(1) Due to the limited reliability of the calculated $\rho\,(\mathbf{k} + \mathbf{G})$ and $\varepsilon\,(\mathbf{k} + \mathbf{G})$, a reliable interpretation of the absolute values of these quantities is hardly possible; it is more realistic to interpret their momentum dependence (even if the spectra are normalized to the total annihilation data).

(2) Especially, the relative enhancement factor in the higher-momentum region, $\varepsilon(\mathbf{k} + \mathbf{G})$ will be of limited reliability in the case when either densities are small or values of the enhancement are close to unity—then resolving whether there is overenhancement or deenhancement does not make sense, the more so, as there is outside of the limit of the experimental possibilities.

(3) Could we compare total annihilation rates?—probably yes because both positron and electron wave functions are normalized to unity. So, for two different approximations, $\rho^{\mathrm{IPM}}(\mathbf{p})$ as a function of $\mathbf{p}$ fluctuates around some fixed value (the true value is always unknown). Here, one should remember the Bunikowski-Schwarz inequality—for each of the IPM models, this norm $||\psi_+\phi_{\mathbf{k}j}|| \leqslant ||\psi_+||\,||\phi_{\mathbf{k}j}||$ could have some other value. However, one could expect that relative differences for total annihilation rates would be smaller than for the corresponding values of $\rho(\mathbf{p})$.

## V. EXPERIMENTAL e-p MOMENTUM DENSITIES

In ACAR experiments, one measures line or plane projections of the e-p momentum densities in the extended $\mathbf{p}$ space, so-called 2D or one-dimensional (1D) spectra. Usually, the experimental results are interpreted from the point of view of the FS studies, so their analysis is limited to the reduced $\mathbf{k}$ space where the FS breaks are better marked. In most cases, they are sufficiently intense to reveal the FS topology,[42,43] although sometimes a presence of the positron does not allow for a proper interpretation of experimental $\rho(\boldsymbol{k})$ without corresponding theoretical calculations.[44] In part (b) of Fig. 2 in Ref. 44, it is shown that, in the case when 5$f$ electrons in $UGa_3$ are treated as a valence ones, there is a very large difference between electron occupancy and theoretical e-p densities $\rho(\mathbf{k})$ (not only can some FS breaks be completely distorted, but also very strong enhancement of some delocalized states can simulate nonexisting FS elements).

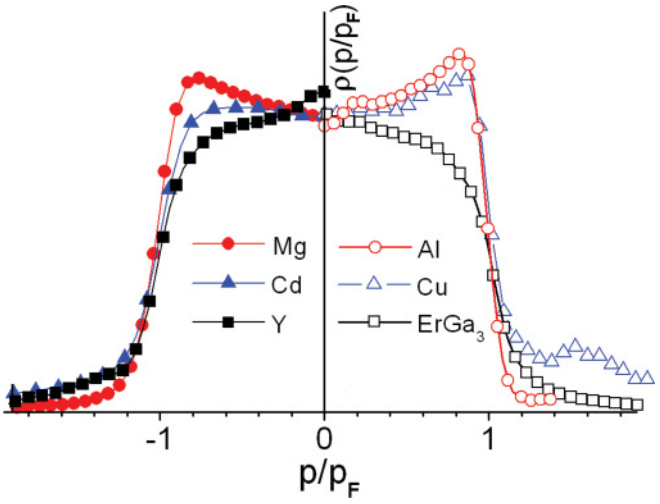


FIG. 8. (Color online) Three-dimensional densities $\rho(\mathbf{p})$ reconstructed from 2D ACAR data for hcp Mg, Cd, and Y along the $\Gamma M$ direction[4] (and references therein) and for cubic metals Al,[45] Cu,[46] and $ErGa_3$ (Ref. 47) along [111] (Al), [100] (Cu), and isotropic average over the 3D $\mathbf{p}$ space in the case of $ErGa_3$.

Of course, to get reliable physical information about correlation effects, one should perform the analysis in the extended zone $\mathbf{p}$ [as well as for three-dimensional (3D) densities, not for 2D ACAR data, to have separated states $\mathbf{k}$ and $\mathbf{k} + \mathbf{G}$], even if the analysis is restricted to momenta inside the central FS. In Fig. 8, we show some examples of 3D densities reconstructed from experimental 2D ACAR data for hcp Mg, Cd, and Y (Ref. 4 and references therein) and for cubic metals Al,[45] Cu,[46] and $ErGa_3$ (Ref. 47) where (1) Mg and Al are "jellium-like" metals with four and three $s$ electrons (per unit cell), respectively; (2) Cd with ten very flat 4$d$ bands lying below the bottom of the 5$s$ conduction bands and Cu with five 3$d$ bands lying closer to the FS (but also without any direct influence on the FS); (3) Y and $ErGa_3$, "real" transition metals with six ($s + d = 4 + 2$) and twelve ($s + p + d = 8 + 3 + 1$) valence electrons in Y and $ErGa_3$, respectively.

As follows from the experimental data, there is typical *Kahana-like* enhancement in simple metals as, e.g., Al, Mg, and Cu (see also results: Al,[29,48] Cu,[49–51] K, Na, Mg, and Al in Ref. 52), a significantly weaker effect for Cd, whereas, e.g., Y and $ErGa_3$, there is no increase in the enhancement with increasing momentum. Only the BML theory[14] is able to describe such different types of enhancement within *one* theory,

which indicates that a proper description of e-p correlations in crystals has to include periodic lattice potentials. Such a finding is important because all other theories ignore the influence of the lattice potential on the e-p interaction. Of course, as we pointed out before, the BML theory has several shortcomings as well as it includes some approximations, which give strong deenhancement in the high-momentum region, up to now not confirmed by the experiment. Similarly, as in the case of Mg,[4] a very detailed interpretation of the 1D ACAR data in Cu (Ref. 49) as well as in Na (Ref. 53) points out that there is no deenhancement of the Umklapp components. Due to this reason, efforts to develop model functions, including empirical enhancement factors as proposed lately by Laverock *et al.*,[17] might be useful. However, it should be performed in the **p** space, and such enhancements cannot be treated as a correction to the theory of the e-p interaction alone but to the theory of both e-p and e-e correlations.

Our explanation is the following. Assume that $\varepsilon^{\mathrm{LDA}}$ in Fig. 3 represents the ratio of experimental-to-theoretical IPM densities. We can try to fit, to the experimental densities, a function simply written in the form $[1 + AE(k)]$, where $A$ is a fitting parameter and $E(k)$ is the energy for the upper band. Since $A$ should describe the dependence on the energy, which is the same in each of the states $\mathbf{k}$, $\mathbf{k} + \mathbf{G}_1$, and $\mathbf{k} + \mathbf{G}_2$, such a procedure would make sense when, for each of these states, we obtained the same parameter $A$. However, performing this for $\varepsilon^{\mathrm{LDA}}$ (the results of the theory where only energy-dependent enhancement was applied,[49,54] although in a local way[27]), we get different $A(\mathbf{G})$ parameters for the leading term and each of the Umklapp components of momentum densities.

When performing such a fitting in the **k** space (in the reduced zone), one gets some effective parameter $A$ that is an average of $A(\mathbf{G})$ with weights depending on the contribution of particular density components to the total density. What is the physical meaning of such a parameter? If it had to show a dependence on the energy, it would make sense only for the leading term of the density.

This feature could also be understood if looking at $\varepsilon^{\mathrm{IPM}}$ in Fig. 3. For each of the Umklapp components, it is strongly momentum dependent, and this is not the case for the leading term of the density. What does it mean? The momentum dependence of the leading term is weakly (compared with Umklapp components) influenced by the **r** dependence of various physical effects, in this case, the positron wave function, i.e., the repulsion of the positron from the positive ions. So, when the energy-dependent enhancement is fitted to the leading term of the density (this is possible only in the **p** space), then it could describe the dependence on the energy.

## VI. CONCLUSIONS

It is demonstrated that, in the periodic lattice, the shape of the positron distribution and the locality of the correlation effects have a crucial influence on the momentum dependence of the e-p densities. It is shown that the positron generally reduces the intensity of electron Umklapp components. The strength of this effect depends on the character of the bands being stronger for localized states. Due to this fact, $\rho(\mathbf{p})$, folded into the first Brillouin zone, does not resemble the steplike function as in the case of electronic densities, and its momentum dependence does not necessarily reflect the dependence of the correlation factor on the momentum or energy. This is, to a large extent, caused by a dependence of the correlation function on the electron density and on the lattice effects (inter- or intraband transitions as in BML theory).

We also showed that, in real metals, due to various effects connected with the spatial inhomogeneities of the materials—static and dynamic lattice effects—many-body tails may be significantly less suppressed than in the jellium. We expect that, due to the same reasons, the momentum densities for $p < p_F$ are decreased. This should, in total, lead to a smoothing out of the momentum density distribution. Such an effect, similar to e-e correlations observed in Compton-scattering measurements, was lately found in new ACAR experiments.[4–8] Such a finding is important because almost all theories dealing with the e-p enhancements assume, according to Carbotte and Kahana,[3] that high-momentum tails are, in practice, to be negligible.

When investigating correlation effects, we have had to ascertain that the momentum dependence of $\rho^{\mathrm{IPM}}(\mathbf{p})$ can be estimated with sufficiently high accuracy, largely independent of approximations of both electron and positron wave functions. We showed that, in the case of "stable" densities (i.e., densities which could be properly estimated from experimental data), the momentum dependence of theoretical IPM densities are only weakly (or, at least, not significantly) dependent on different band-structure calculations. In fact, we do not consider such different band-structure calculations as in the paper.[39] We assume that their level is adequately high to describe the FS properly; if not, one cannot perform any analysis of $\rho(\mathbf{p})$. But even when the band-structure method allows for obtaining the proper FS, one cannot go into such subtle details as the absolute values of densities. Therefore, one should restrict the analysis to relative changes in $\rho(\mathbf{p})$ as well as to such regions where $\rho(\mathbf{p})$ could be estimated with sufficiently high accuracy [more details are points (1)–(3) at the end of Sec. IV]. Then, one could devote all differences, arising in various theoretical results, to different models for many-body effects.

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