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# The sensitivity of electron–positron momentum densities to approximations used in calculating the positron wave function

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**Abstract.** In this paper, the behaviour of the electron–positron momentum density of non-interacting particles, $\rho^{\mathrm{IPM}}(\boldsymbol{p})$, in a periodic lattice potential is investigated. On the basis of general considerations, we show that in each metal there are some components of $\rho^{\mathrm{IPM}}(\boldsymbol{p})$ which are only weakly sensitive to approximations used in the calculation of the positron wave function $\psi_{+}(\boldsymbol{r})$. This means that in these regions of $\boldsymbol{p}$, the two-particle density $\rho^{\mathrm{IPM}}(\boldsymbol{p})$ can be evaluated with a high accuracy, largely independently of uncertainties arising from the different approximations used in calculating the function $\psi_{+}(\boldsymbol{r})$. This property of $\rho^{\mathrm{IPM}}(\boldsymbol{p})$ can be useful for the verification of various approaches used for describing the electron–positron interaction in real metals.

## 1. Introduction

In experiments using the angular correlation of positron annihilation radiation (ACPAR) technique, one measures linear (or planar) integrals of the momentum density of electron–positron annihilation pairs (MDAP), $\rho(\boldsymbol{p})$. It is well known that the annihilation process is strongly influenced by the Coulomb interaction between the electrons and the positron. Theoretically, this influence can be described by a momentum-dependent enhancement factor $\epsilon(\boldsymbol{p})$ which is defined as the ratio of the real momentum density and the density within the independent-particle model (IPM):

$$\epsilon(\boldsymbol{p}) = \rho(\boldsymbol{p})/\rho^{\mathrm{IPM}}(\boldsymbol{p}) \tag{1}$$

where, in the IPM, the interaction of the annihilating fermions is completely ignored.

The enhancement of the annihilation rate has been intensively studied for the jellium model (for reviews see [1–3]). However, there are still problems concerning a description of the enhancement effect in realistic systems, i.e. for the inhomogeneous electron gas found in real metals. Here various theoretical approaches have been proposed (for reviews see [1–5]) which lead to different results for $\epsilon(\boldsymbol{p})$, especially for the higher-momentum components (HMC) of the momentum density distribution [6–18].

To decide which theoretical approach describes reality more closely, careful comparisons of theoretically and experimentally obtained MDAP results are necessary. Of course, such

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a comparison requires a precise calculation of $\rho^{\mathrm{IPM}}(\boldsymbol{p})$ as well as a precise analysis of the experimental data [19–24]. However, as has been shown in [19–21], the HMC densities are generally remarkably sensitive to details of the calculations, such as the crystal potentials used and the accuracy of the positron wave function. Nevertheless, as has been shown by Sormann and Šob for the alkali metals (bcc structure) [19] and for Cu and Pd (fcc structure) [21], this sensitivity of the MDAP is weak for the HMC which lie close to the centre of the momentum space. Moreover, Daniuk *et al* [23] obtained the result that total annihilation rates are also only weakly sensitive to details of the calculation of the positron wave function $\psi_+(\boldsymbol{r})$.

In the present paper which is based on the theory proposed in [4], we explain numerical results from the literature [19–24]. Beyond that, the theory presented in section 2 is even more general, showing that for each metal and for each electron state $\boldsymbol{k}j$ there exist at least two components of $\rho^{\mathrm{IPM}}(\boldsymbol{p})$ which are only weakly sensitive to approximations used in evaluating the positron wave function, namely the leading density component (the density of the highest value) and at least one dominant Umklapp component. Moreover, our theory also shows that the higher the value of the Umklapp density, the smaller this sensitivity is, which is remarkable because it is just these 'stable' densities that can be really studied experimentally. This property of the MDAP is important for a reliable verification of various approaches used for a theoretical description of the electron–positron interaction, because if we compare experimental and theoretical annihilation rates especially for the Umklapp components we have no need to be concerned that eventual disagreements between theory and experiment may be connected with erroneous IPM rate calculations due to uncertainties arising from approximations used in calculating the positron wave function.

In this context it should be emphasized that there is, of course, no actual necessity to use approximative positron wave functions in IPM rate calculations. In fact, there exist rate formulae which take into account the full spatial anisotropy of $\psi_+$—for example the formula based on the Korringa–Kohn–Rostoker (KKR) method and a multiple-scattering formalism [25–27]. Nevertheless, many authors whose positron work is based on the augmented-plane-wave (APW) formalism (or other related formalisms) use simplifications of $\psi_+$ involving a partial or total neglect of its spatial anisotropy. The reason for this is that the APW rate formula including the fully anisotropic positron wave function leads to mathematical expressions which are too complicated for many practical purposes [28, 29].

## 2. Theory

The momentum density of a non-interacting electron–positron pair (within a periodic lattice) for the momentum $\boldsymbol{k}+\boldsymbol{G}$ and state $\boldsymbol{k}j$ reads

$$\rho_j^{\mathrm{IPM}}(\boldsymbol{k}+\boldsymbol{G}) = n(\boldsymbol{k}j)\left|\int_\Omega \mathrm{d}^3r\ \psi_+(\boldsymbol{r})\phi_{\boldsymbol{k}j}(\boldsymbol{r})\exp[-\mathrm{i}(\boldsymbol{k}+\boldsymbol{G})\cdot\boldsymbol{r}]\right|^2. \tag{2}$$

$\psi_+(\boldsymbol{r})$ describes the wave function of the thermalized positron, and $\phi_{\boldsymbol{k}j}(\boldsymbol{r})$ is the wave function of a Bloch electron with (reduced) Bloch vector $\boldsymbol{k}$ in the $j$th band. $\boldsymbol{G}$ is a reciprocal-lattice vector, $\Omega$ is the volume of the crystal and $n(\boldsymbol{k}j)$ denotes the occupation number (0 or 1) in the state $\boldsymbol{k}j$. Due to the Bloch property of the wave functions, this density (henceforth, the superscript IPM will be omitted) can be expressed as

$$\rho_j(\boldsymbol{k}+\boldsymbol{G}) = n(\boldsymbol{k}j)\left|\sum_{\boldsymbol{H}} u_{\boldsymbol{k}j}(\boldsymbol{H})v(\boldsymbol{G}-\boldsymbol{H})\right|^2 \tag{3}$$

where $\boldsymbol{H}$ is also a reciprocal-lattice vector, and $u_{\boldsymbol{k}j}$ and $v$ are the coefficients of the Fourier expansions of the functions $\phi_{\boldsymbol{k}j}$ and $\psi_+$, respectively. According to [4], the electron–positron densities $\rho_j$ can be written as

$$\rho_j(\boldsymbol{k}+\boldsymbol{G}) = n(\boldsymbol{k}j)|u_{\boldsymbol{k}j}(\boldsymbol{G}_{\boldsymbol{k}j})|^2|v(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j})|^2\left[1+\alpha_{\boldsymbol{k}j}(\boldsymbol{G})\right]^2 \tag{4}$$

where

$$\alpha_{\boldsymbol{k}j}(\boldsymbol{G}) = \sum_{\boldsymbol{H}\neq\boldsymbol{G}_{\boldsymbol{k}j}} \frac{v(\boldsymbol{G}-\boldsymbol{H})u_{\boldsymbol{k}j}(\boldsymbol{H})}{v(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j})u_{\boldsymbol{k}j}(\boldsymbol{G}_{\boldsymbol{k}j})} \tag{5}$$

with $\boldsymbol{G}_{\boldsymbol{k}j}$ as the reciprocal-lattice vector belonging to the 'leading' Fourier coefficient of the electron wave function with the property $|u_{\boldsymbol{k}j}(\boldsymbol{G}_{\boldsymbol{k}j})| > |u(\boldsymbol{H})|$. As one can see from equation (4), $\boldsymbol{G} = \boldsymbol{G}_{\boldsymbol{k}j}$ refers the main contribution of the electron–positron momentum density (with the electron in the state $\boldsymbol{k}j$), whereas all vectors $\boldsymbol{G} \neq \boldsymbol{G}_{\boldsymbol{k}j}$ belong to Umklapp components of this density.

In the following investigation, we shall focus our attention on the question of how sensitively the density $\rho_j(\boldsymbol{k}+\boldsymbol{G})$ reacts to different approximations used in calculating the positron wave function. For this purpose, we start with the following definitions.

First, we define $\Delta\rho_+(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j})$ as the relative difference of the squares of the Fourier coefficients belonging to a chosen reciprocal-lattice vector $\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j}$ for two models of $\psi_+$, namely $\psi_+^{(m)}$ and $\psi_+^{(l)}$, where the indices $(m)$ and $(l)$ are used in such a way that $|v^{(m)}(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j})| > |v^{(l)}(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j})|$ is valid. Then, $\Delta\rho_+(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j})$ is described by the positive quantity

$$\Delta\rho_+(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j}) = \frac{\left[v^{(m)}(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j})\right]^2 - \left[v^{(l)}(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j})\right]^2}{\left[v^{(l)}(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j})\right]^2} = \left[\frac{v^{(m)}(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j})}{v^{(l)}(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j})}\right]^2 - 1. \tag{6}$$

Secondly, we define the sensitivity $\Delta\rho_j(\boldsymbol{k}+\boldsymbol{G})$ of the electron–positron density for the (occupied) electron state $\boldsymbol{k}j$ within the Brillouin zone centred around the reciprocal-lattice vector $\boldsymbol{G}$, also with respect to different models of the positron wave function. We define this positive quantity $\Delta\rho_j(\boldsymbol{k}+\boldsymbol{G})$ by the expression

$$\Delta\rho_j(\boldsymbol{k}+\boldsymbol{G}) = |\rho_j^{(m)}(\boldsymbol{k}+\boldsymbol{G}) - \rho_j^{(l)}(\boldsymbol{k}+\boldsymbol{G})|/\min\left\{\rho_j^{(m)};\, \rho_j^{(l)}\right\}. \tag{7}$$

Combining equations (7) and (4), $\Delta\rho_j$ can be written in the form

$$\Delta\rho_j(\boldsymbol{k}+\boldsymbol{G}) = \left\{\left[\frac{v^{(m)}(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j})}{v^{(l)}(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j})}\right]\left[1+\kappa_{\boldsymbol{k}j}^{(l,m)}(\boldsymbol{G})\right]\right\}^{2n} - 1 \tag{8}$$

where $n = +1$ for $\rho_j^{(m)} > \rho_j^{(l)}$ and $n = -1$ for $\rho_j^{(m)} < \rho_j^{(l)}$. Here it is important to emphasize that for $|v^{(m)}(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j})| > |v^{(l)}(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j})|$, $\rho_j^{(m)}(\boldsymbol{k}+\boldsymbol{G})$ can be either greater or smaller than $\rho_j^{(l)}(\boldsymbol{k}+\boldsymbol{G})$. The quantity $\kappa_{\boldsymbol{k}j}$ which occurs in expression (8) is given by

$$\kappa_{\boldsymbol{k}j}^{(l,m)}(\boldsymbol{G}) = \left[\alpha_{\boldsymbol{k}j}^{(m)}(\boldsymbol{G}) - \alpha_{\boldsymbol{k}j}^{(l)}(\boldsymbol{G})\right] \Big/ \left[1+\alpha_{\boldsymbol{k}j}^{(l)}(\boldsymbol{G})\right]. \tag{9}$$

Here $\alpha^{(i)}$ for $i = l$ or $i = m$ is given by equation (5) with $v(\boldsymbol{G})$ replaced by $v^{(i)}(\boldsymbol{G})$. As can be seen from equation (8), the sensitivity $\Delta\rho_j$ depends on the ratio of particular Fourier coefficients belonging to different approximations used in calculating the positron wave function, and on the quantity $\kappa_{\boldsymbol{k}j}$ given by equation (9) whose behaviour is—as will be shown later—mainly determined by the Fourier coefficients $u_{\boldsymbol{k}j}(\boldsymbol{G})$ of the electron wave function in the state $\boldsymbol{k}j$.

On comparing equations (8) and (6), it is obvious that there are strong connections between the quantities $\Delta\rho_j(\boldsymbol{k}+\boldsymbol{G})$ and $\Delta\rho_+(\boldsymbol{G}-\boldsymbol{G}_{kj})$. In fact, it is one of the main purposes of this paper to find these connections. Therefore, we finally define the quantity $y$ which is given by the positive ratio

$$y(\kappa_{kj}) = \Delta\rho_j(\boldsymbol{k}+\boldsymbol{G})/\Delta\rho_+(\boldsymbol{G}-\boldsymbol{G}_{kj}). \tag{10}$$

To facilitate the reading of the formulae in the following sections, the index $j$ in $\rho_j(\boldsymbol{k}+\boldsymbol{G})$ and the index $\boldsymbol{k}j$ in $\alpha_{kj}$, $\kappa_{kj}$ and $u_{kj}$ will be omitted from now on.

### *2.1. The parameters α and κ*

Before we start to study the relations between $\Delta\rho$ and $\Delta\rho_+$, we will estimate the quantities $\alpha(\boldsymbol{G})$ and $\kappa(\boldsymbol{G})$, considering the two cases $\boldsymbol{G}=\boldsymbol{G}_{kj}$ and $\boldsymbol{G}\neq\boldsymbol{G}_{kj}$ separately.

As it was shown in [4], for $\boldsymbol{G}=\boldsymbol{G}_{kj}$, the application of Abel's lemma to equation (5) allows us to express $\alpha(\boldsymbol{G}_{kj})$ via

$$\alpha^{(i)}(\boldsymbol{G}_{kj}) = \frac{x^{(i)}}{u(\boldsymbol{G}_{kj})}\max_{[\boldsymbol{H}\neq\boldsymbol{G}_{kj}]}|u(\boldsymbol{H})| \qquad (i=m,l) \tag{11}$$

where $|x^{(i)}|\leqslant 1$, i.e. $\alpha^{(i)}(\boldsymbol{G}_{kj})$ is always considerably smaller than 1 (in appendix A of [4], in equation (A6), it should read $\alpha(\boldsymbol{G}_{kj})$ instead of $\alpha(\boldsymbol{G})$). Using equations (9) and (11), one gets

$$\kappa^{(l,m)}(\boldsymbol{G}_{kj}) = \left[\frac{x^{(m)}}{x^{(l)}}-1\right]\frac{1}{1+1/\alpha^{(l)}(\boldsymbol{G}_{kj})}. \tag{12}$$

For an estimation of the ratio $x^{(m)}/x^{(l)}$, we combine equations (5) and (11), obtaining the sums

$$S^{(i)} = \sum_{\boldsymbol{H}\neq\boldsymbol{G}_{kj}} v^{(i)}(\boldsymbol{G}_{kj}-\boldsymbol{H})u(\boldsymbol{H}) = x^{(i)}v^{(i)}(\boldsymbol{0})\max_{[\boldsymbol{H}\neq\boldsymbol{G}_{kj}]}|u(\boldsymbol{H})|$$

with $i=m$ or $l$. Then we have

$$S^{(l,m)} \equiv S^{(m)}-S^{(l)} = \left[\frac{x^{(m)}v^{(m)}(\boldsymbol{0})}{x^{(l)}v^{(l)}(\boldsymbol{0})}-1\right]S^{(l)} \approx \left[\frac{x^{(m)}}{x^{(l)}}-1\right]S^{(l)}$$

where the last (approximative) identity follows from the fact that the first Fourier coefficient of the positron wave function changes slightly with the model used, i.e. $v^{(m)}(\boldsymbol{0})\approx v^{(l)}(\boldsymbol{0})$ (see section 2.3). However, $S^{(l,m)}$ can also be considered as the sum

$$\sum_{\boldsymbol{H}\neq\boldsymbol{G}_{kj}}\left[v^{(m)}(\boldsymbol{G}_{kj}-\boldsymbol{H})-v^{(l)}(\boldsymbol{G}_{kj}-\boldsymbol{H})\right]u(\boldsymbol{H}).$$

Provided that (i) the Fourier coefficients of $\psi_+$ for the first reciprocal-lattice vectors, which give the largest contribution to the sum $S^{(i)}$, are only weakly dependent on the approximations used in calculating $\psi_+$, and (ii) $\sum_{\boldsymbol{G}} v(\boldsymbol{G}) = 0$, one could expect that $|S^{(l,m)}| \ll |S^{(l)}|$. This leads to the condition that $|x^{(m)}/x^{(l)}-1| \ll 1$. Taking this into account together with the fact that $\alpha(\boldsymbol{G}_{kj})$ is small, equation (12) gives the general result

$$|\kappa(\boldsymbol{G}_{kj})| \ll 1. \tag{13}$$

For $\boldsymbol{G}\neq\boldsymbol{G}_{kj}$, corresponding to Umklapp components of $\rho(\boldsymbol{k}+\boldsymbol{G})$, it is convenient to write equation (5) in the form

$$\alpha^{(i)}(\boldsymbol{G}) = \frac{1}{v^{(i)}(\boldsymbol{G}-\boldsymbol{G}_{kj})u(\boldsymbol{G}_{kj})}\left[u(\boldsymbol{G})v^{(i)}(\boldsymbol{0}) + \sum_{\boldsymbol{H}\neq\boldsymbol{G},\boldsymbol{G}_{kj}} v^{(i)}(\boldsymbol{G}-\boldsymbol{H})u(\boldsymbol{H})\right] \tag{14}$$

with $i = m$ or $l$. The application of Abel's lemma to the second term of this equation leads to the expression

$$\alpha^{(i)}(\boldsymbol{G}) = \frac{v^{(i)}(\boldsymbol{0})}{u(\boldsymbol{G}_{kj})v^{(i)}(\boldsymbol{G}-\boldsymbol{G}_{kj})}\left[u(\boldsymbol{G}) + x^{(i)}u_{\max}\right] \tag{15}$$

with

$$u_{\max} = \max_{[\boldsymbol{H}\neq\boldsymbol{G},\boldsymbol{G}_{kj}]} |u(\boldsymbol{H})|$$

and $|x^{(i)}| < 1$. Inserting this in equation (9), one gets for $\kappa^{(l,m)}$ the form

$$\kappa^{(l,m)}(\boldsymbol{G}) = \left\{\frac{v^{(l)}(\boldsymbol{G}-\boldsymbol{G}_{kj})}{v^{(m)}(\boldsymbol{G}-\boldsymbol{G}_{kj})}\eta^{(l,m)}(\boldsymbol{G}) - 1\right\}\frac{1}{1+1/\alpha^{(l)}(\boldsymbol{G})} \tag{16}$$

where

$$\eta^{(l,m)}(\boldsymbol{G}) = \frac{v^{(m)}(\boldsymbol{0})\left[u(\boldsymbol{G}) + x^{(m)}u_{\max}\right]}{v^{(l)}(\boldsymbol{0})\left[u(\boldsymbol{G}) + x^{(l)}u_{\max}\right]} \tag{17}$$

and

$$\alpha^{(m)}(\boldsymbol{G}) = \eta^{(l,m)}(\boldsymbol{G})\alpha^{(l)}(\boldsymbol{G})\frac{v^{(l)}(\boldsymbol{G}-\boldsymbol{G}_{kj})}{v^{(m)}(\boldsymbol{G}-\boldsymbol{G}_{kj})}. \tag{18}$$

Because $v^{(m)}(\boldsymbol{0}) \approx v^{(l)}(\boldsymbol{0})$, the quantity $\eta^{(l,m)}$ is close to unity except when $|u(\boldsymbol{G})+x^{(i)}u_{\max}|$ takes such small values that the difference between $x^{(m)}$ and $x^{(l)}$ dominates the quotient in equation (17). $\eta^{(l,m)} = 1$ means that $\kappa^{(l,m)}$ (and also $\Delta\rho$) depends only on the change in the particular $v(\boldsymbol{G}-\boldsymbol{G}_{kj})$ coefficient (see equations (8) and (16)). When $\eta^{(l,m)} \neq 1$, $\kappa^{(l,m)}$ and $\Delta\rho$ depend on the changes of all of the Fourier coefficients of the positron wave function.

Henceforth, such Umklapp components, for which the density has the property

$$\rho(\boldsymbol{k}+\boldsymbol{G}) > |u(\boldsymbol{G}_{kj})|^2|v(\boldsymbol{G}-\boldsymbol{G}_{kj})|^2$$

but also $|u(\boldsymbol{G})+xu_{\max}|$ is not close to zero (which means that $\alpha$ cannot be close to zero), will be called *relevant* components. So, for *relevant* components, we have $\alpha > 0$ or $\alpha < -2$ (see equation (4)) as well as $\eta^{(l,m)}$ being close to unity. We should point out that all densities of remarkably high value which can be recognized in the experiment belong to *relevant* components. The opposite statement is not true—i.e. some *relevant* components can have a small value if $v(\boldsymbol{G}-\boldsymbol{G}_{kj})$ is small.

### *2.2. The behaviour of the function $y(\kappa)$*

As we emphasized before, the function $y$ which has been introduced by equation (10) plays a central role in our investigation. It is therefore important to have a good knowledge about this function, especially as regards its dependence on the quantity $\kappa^{(l,m)}$ defined by equation (16). This dependence can be directly obtained by the use of equations (6), (8) and (10), and the functional relations between $\alpha^{(m)}$, $\alpha^{(l)}$ and $\kappa^{(l,m)}$ can be derived by using equations (16)–(18).

To make the following formulae more readable, henceforth all $v^{(m)}$ and $v^{(l)}$ given without an argument mean $v^{(m)}(\boldsymbol{G}-\boldsymbol{G}_{kj})$ and $v^{(l)}(\boldsymbol{G}-\boldsymbol{G}_{kj})$, respectively.

The typical behaviour of $y$ is given in figure 1 where we show this function for $v^{(m)}/v^{(l)} = 1.5$ which corresponds to $\Delta\rho_+ = 1.25$. Special (negative) values of $\kappa^{(l,m)}$ for which $y = 0$ or 1 (see figure 1) are as follows:

$$\begin{aligned} &\kappa_1^{(l,m)} = |v^{(l)}/v^{(m)}| - 1 \qquad \text{and} \qquad \kappa_2^{(l,m)} = (v^{(l)}/v^{(m)})^2 - 1 \\ &\kappa_3^{(l,m)} = -(v^{(l)}/v^{(m)})^2 - 1 \qquad \text{and} \qquad \kappa_4^{(l,m)} = -|v^{(l)}/v^{(m)}| - 1. \end{aligned} \tag{19}$$

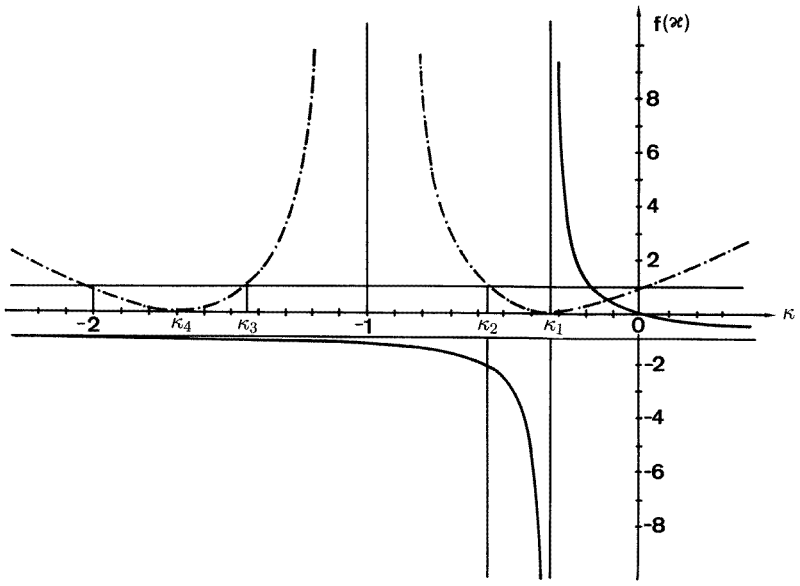


**Figure 1.** $y(\kappa)$ and the average value of $\alpha(\kappa) = (\alpha^{(m)} + \alpha^{(l)})/2$ for $v^{(m)}/v^{(l)} = 1.5$ and $\eta^{(l,m)} = 1$ are represented by chain and full curves, respectively. $\kappa$ denotes $\kappa^{(l,m)}$.

This figure also shows $\alpha$ as a function of $\kappa^{(l,m)}$. For the parameter $\eta^{(l,m)}$ (equation (17)), we chose the value 1 because $\eta^{(l,m)} \approx 1$ is typical for *relevant* Umklapp components (see section 2.1). In this case, the functional behaviour of $\alpha^{(m)}$ and $\alpha^{(l)}$ is similar, and therefore we only present the mean values of $\alpha^{(m)}$ and $\alpha^{(l)}$. Now, we shall focus our attention on those regions of $\kappa^{(l,m)}$ where $y < 1$ which is—according to figure 1—obviously the case for $-2 \leqslant \kappa^{(l,m)} \leqslant \kappa_3$ and for $\kappa_2 \leqslant \kappa^{(l,m)} \leqslant 0$. We see that for the first of these two regions, both $\alpha^{(m)}$ and $\alpha^{(l)}$ are close to –1. According to equation (4), such values of $\alpha$ belong to small (i.e. *non-relevant*) components of $\rho(\boldsymbol{k} + \boldsymbol{G})$ which are of no interest for our studies. For the second region of $\kappa^{(l,m)}$ where $y$ is smaller than 1, the corresponding $\alpha^{(m)}$- and $\alpha^{(l)}$-values obey the relations

$$\alpha^{(i)}(\boldsymbol{G}) > 0 \qquad (i = m, l) \tag{20}$$

and, according to equations (16)–(18),

$$\alpha^{(l)}(\boldsymbol{G}) < -\left[1 + v^{(m)}/v^{(l)}\right] \qquad \text{and} \qquad \alpha^{(m)}(\boldsymbol{G}) < -\left[1 + v^{(l)}/v^{(m)}\right]. \tag{21}$$

Additionally, as can be directly derived from equations (16) and (18), for $v^{(m)}/v^{(l)} > 0$ and for $\eta^{(l,m)} = 1$, both $\alpha^{(m)}(\kappa)$ and $\alpha^{(l)}(\kappa)$ have the same vertical asymptote for $\kappa = \kappa_1$.

Therefore, we can say that in the region $\kappa_2 \leqslant \kappa^{(l,m)} \leqslant 0$ where we have $y < 1$, the values of $\alpha$ are either positive (equation (20)) or they are at least approximately smaller than –2, provided that $|v^{(m)}/v^{(l)}|$ is not too different from 1 (see equation (21)). This is one of the most important results of this paper, because it means that we can be sure that, for all *relevant* Umklapp densities, $y$ will be smaller than 1, i.e. $\Delta\rho_+(\boldsymbol{G} - \boldsymbol{G}_{kj})$ represents an upper limit for $\Delta\rho(\boldsymbol{k} + \boldsymbol{G})$.

In figure 2(a), we also show $\left(\alpha^{(m)} + \alpha^{(l)}\right)/2$ as a function of $\kappa^{(l,m)}$, also for $v^{(m)}/v^{(l)}$ = 1.5, but for two different values of $\eta^{(l,m)} \neq 1$, namely for 1.05 and for 0.952. In these cases, as previously mentioned, $\Delta\rho$ depends on the change of all of the Fourier coefficients

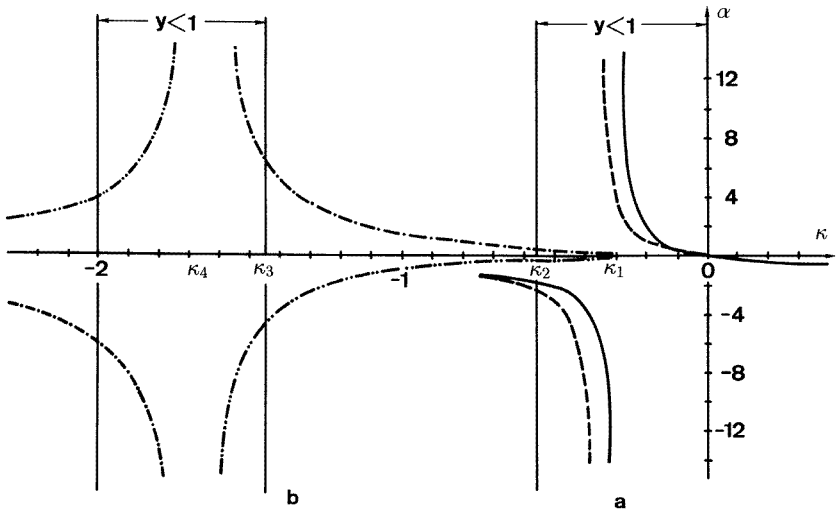


**Figure 2.** (a) $\alpha = (\alpha^{(m)} + \alpha^{(l)})/2$ as a function of $\kappa^{(l,m)}$, corresponding to $v^{(m)}/v^{(l)} = 1.5$, is given by full and broken curves for $\eta^{(l,m)} = 1.05$ and 0.952, respectively. (b) $\alpha^{(l)}$ and $\alpha^{(m)}$ for $\eta^{(l,m)} = 1$ and $v^{(m)}/v^{(l)} = -1.5$ are shown by broken–dotted and broken–double-dotted curves, respectively.

of $\psi_+$, and the position of the vertical asymptote of $\alpha$ (hereafter called $\kappa_P$) will no longer coincide with $\kappa_1$. For example, for $\eta^{(l,m)} > v^{(m)}/v^{(l)}$, $\kappa_P$ is greater than zero and, as a consequence, for all positive values of $\alpha$, we have $y > 1$ and, therefore,

$$\Delta\rho(\boldsymbol{k}+\boldsymbol{G}) > \Delta\rho_+(\boldsymbol{G}-\boldsymbol{G}_{kj}).$$

However, such high values of $\eta^{(l,m)}$ are never connected with *relevant* components of $\rho(\boldsymbol{k}+\boldsymbol{G})$.

For $v^{(l)}/v^{(m)} < \eta^{(l,m)} < 1$ and $1 < \eta^{(l,m)} < v^{(m)}/v^{(l)}$, $\kappa_P$ is smaller or greater than $\kappa_1$, respectively, but it is always a negative number, and the condition $y < 1$ is satisfied for all positive values of $\alpha$ and also for all negative $\alpha$ which are connected with *relevant* components of the density.

The appearance of small values of $y$ for $\kappa \approx \kappa_1$ can also be considered in the following way: for very high values of $|\alpha|$, one obtains using equations (4) and (15) that

$$\rho^{(i)}(\boldsymbol{k}+\boldsymbol{G}) \approx |v^{(i)}(\boldsymbol{0})|^2 |u(\boldsymbol{G}) + x^{(i)} u_{\max}|^2 \tag{22}$$

with $u_{\max}$ as defined in section 2.1. Consequently, using equations (8) and (16), one gets

$$\Delta\rho(\boldsymbol{k}+\boldsymbol{G}) \approx \left[\eta^{(l,m)}\right]^{2n} - 1 \tag{23}$$

($n = +1$ for $\rho^{(m)} > \rho^{(l)}$ and $n = -1$ for $\rho^{(m)} < \rho^{(l)}$) which means that $\Delta\rho(\boldsymbol{k}+\boldsymbol{G})$ is no longer dependent on the Fourier coefficients of the positron wave function for $\boldsymbol{G}-\boldsymbol{G}_{kj}$. Taking into account that $\eta^{(l,m)}$ is close to unity for all *relevant* components, we find that $\Delta\rho(\boldsymbol{k}+\boldsymbol{G})$ is close to zero.

Figure 2(b) shows the behaviour of $\alpha$ in connection with a change of sign of $v(\boldsymbol{G}-\boldsymbol{G}_{kj})$ for different models of $\psi_+$. This can only happen for very small Fourier coefficients of the positron wave function belonging to large vectors $\boldsymbol{G}-\boldsymbol{G}_{kj}$. Of course, if the corresponding density is to be a *relevant* one, $|\alpha|$ must also be large, and—as seen from this figure—for such $|\alpha|$, $y$ is less than 1.

Finally, we return to a discussion of the particular case of the leading components of the density, i.e. for $\boldsymbol{G} = \boldsymbol{G}_{kj}$. It follows from the argumentation of section 2.1 that $\kappa(\boldsymbol{G}_{kj})$ is small with respect to 1 but might be positive or negative. Due to this, $\Delta\rho_+(\boldsymbol{0})$ cannot be reliably considered as an upper limit of $\Delta\rho(\boldsymbol{k}+\boldsymbol{G}_{kj})$ because of the fact that $y$ could be greater than 1. However, because both quantities $\kappa(\boldsymbol{G}_{kj})$ and $\Delta\rho_+(\boldsymbol{0})$ are small, the changes in the leading component of the density are small, too (see equation (8)).

Here we would like to point out an important property of $\Delta\rho$. If the lattice effects are small, i.e. if $u(\boldsymbol{G}_{kj})$ strongly dominates over all other Fourier coefficients of the electron wave function, then we learn from equation (11) that $\alpha(\boldsymbol{G}_{kj})$ is a small number. More marked lattice effects could lead to an increase of $|\alpha(\boldsymbol{G}_{kj})|$. Additionally, according to equation (12), $|\kappa(\boldsymbol{G}_{kj})|$ is also an increasing function of $|\alpha(\boldsymbol{G}_{kj})|$. As we already know (compare figure 1), for positive values of $\kappa$, $y > 1$ goes up with $\kappa$, and this increase might be extremely strong especially for small values of $\Delta\rho_+$ (typical for the leading components of $\rho(\boldsymbol{k}+\boldsymbol{G})$). Therefore, in this case, increasing lattice effects could lead to values of $y$ which are significantly higher than 1. In contrast, for *relevant* Umklapp components (the region where $\kappa_2 \leqslant \kappa \leqslant 0$), the opposite can be observed. In this case, as can also be seen from figure 1, an increase of the significance of the lattice effects, i.e. an increase of $|\alpha|$, leads to a decrease of $y$, and $|\alpha| \to \infty$ has the consequence that $\kappa \to \kappa_1$ and $y \to 0$ if $\eta^{(l,m)}$ is close to unity (this always takes place for Umklapp components of high density, as e.g. are found for transition metals). This is important because Umklapp densities of high values are of specific interest for both experimental and theoretical studies—for example, studies of correlation effects.

To end this section it should be noticed that our theory can describe various features of $\rho(\boldsymbol{p})$. For example, one can show that generally, i.e. except for for very specific (particular) changes of both $v(\boldsymbol{G}-\boldsymbol{G}_{kj})$ and $v(\boldsymbol{0})$,

$$\Delta\rho(\boldsymbol{k}+\boldsymbol{G}) > \Delta\rho_+(\boldsymbol{0}).$$

For this purpose let us rewrite equation (4) in the form

$$\rho(\boldsymbol{k}+\boldsymbol{G}) = n(\boldsymbol{k}j)|u(\boldsymbol{G}_{kj})|^2|v(\boldsymbol{0})|^2\,[1+\beta(\boldsymbol{G})]^2$$

where

$$\beta(\boldsymbol{G}) = -1 + \frac{v(\boldsymbol{G}-\boldsymbol{G}_{kj})}{v(\boldsymbol{0})} + \frac{u(\boldsymbol{G})}{u(\boldsymbol{G}_{kj})} + \frac{xu_{\max}}{u(\boldsymbol{G}_{kj})}$$

with $xu_{\max}$ as defined in section 2.1. Taking into account the relationship between $xu_{\max}$ and $\alpha(\boldsymbol{G})$, $\beta(\boldsymbol{G})$ reads

$$\beta(\boldsymbol{G}) = -1 + \frac{v(\boldsymbol{G}-\boldsymbol{G}_{kj})}{v(\boldsymbol{0})}\,[1+\alpha(\boldsymbol{G})]\,. \tag{24}$$

Similarly to the way in which we described $\rho(\boldsymbol{k}+\boldsymbol{G})$ using equation (4), we define $\Delta\rho$ according to the formula (8) where now $v^{(i)}(\boldsymbol{G}-\boldsymbol{G}_{kj})$ and $\kappa^{(l,m)}$ are replaced by $v^{(i)}(\boldsymbol{0})$ and $\tilde{\kappa}^{(l,m)}$, respectively, where

$$\tilde{\kappa}^{(l,m)}(\boldsymbol{G}) = \frac{\beta^{(m)}(\boldsymbol{G}) - \beta^{(l)}(\boldsymbol{G})}{1+\beta^{(l)}(\boldsymbol{G})}. \tag{25}$$

Here we study the relationship between $\Delta\rho(\boldsymbol{k}+\boldsymbol{G})$ and $\Delta\rho_+(\boldsymbol{0})$ which describes the change of the leading Fourier coefficient of the positron wave function, $v(\boldsymbol{0})$. It is given by the same function $y$ (which is defined by equation (10) and presented in figure 1) if $\Delta\rho_+(\boldsymbol{G}-\boldsymbol{G}_{kj})$ in equation (10) is replaced by $\Delta\rho_+(\boldsymbol{0})$, which is usually a small number. All of the expressions for the negative $\kappa_i$ are exactly the same if one resets the $v^{(i)}(\boldsymbol{G}-\boldsymbol{G}_{kj})$ in

equation (19) to $v^{(i)}(\mathbf{0})$. Due to the fact that $\Delta\rho_+(\mathbf{0}) + 1 \approx 1$, we obtain $\tilde{\kappa}_1 \approx \tilde{\kappa}_2 \approx 0$ and $\tilde{\kappa}_3 \approx \tilde{\kappa}_4 \approx -2$. Taking into account that $\tilde{\kappa}^{(l,m)}$ cannot be close to $-2$, the condition $\Delta\rho(\boldsymbol{G}) < \Delta\rho_+(\mathbf{0})$ requires fulfilment of the inequality

$$\frac{v^{(l)}(\mathbf{0})}{v^{(m)}(\mathbf{0})} < \frac{v^{(m)}(\boldsymbol{G}-\boldsymbol{G}_{kj})[1+\alpha^{(m)}(\boldsymbol{G})]}{v^{(l)}(\boldsymbol{G}-\boldsymbol{G}_{kj})[1+\alpha^{(l)}(\boldsymbol{G})]} < \frac{v^{(m)}(\mathbf{0})}{v^{(l)}(\mathbf{0})}$$

which is connected to a specific change of both $v(\boldsymbol{G}-\boldsymbol{G}_{kj})$ and $v(\mathbf{0})$. Therefore, the probability of finding $\Delta\rho(\boldsymbol{G}) < \Delta\rho_+(\mathbf{0})$ is very small.

### *2.3. Changes of the Fourier coefficients of the positron wave function*

Here we study the sensitivity of the Fourier coefficients of the positron wave function $\psi_+(\boldsymbol{r})$ with respect to arbitrarily different approximations. As regards the use of such approximated positron wave functions in IPM rate calculations, see our argumentation in section 1. As an example, let us consider a muffin-tin approximation of $\psi_+$ as was originally proposed by Loucks [30] and has been discussed in detail in [20]:

$$\psi_+^{(\mathrm{L})}(\boldsymbol{r}) = \begin{cases} c & \text{for } |\boldsymbol{r}| > r_{\mathrm{MT}} \\ \psi_{\mathrm{sph}}(r) & \text{for } |\boldsymbol{r}| \leqslant r_{\mathrm{MT}} \end{cases} \tag{26}$$

where $\psi_{\mathrm{sph}}(r)$ is the spherical average of an APW positron wave function inside the muffin-tin sphere with the radius $r_{\mathrm{MT}}$. Outside this sphere, $\psi_+$ is approximated by the constant $c$. Due to this special procedure, $c$ does not coincide with $\psi_{\mathrm{sph}}(r = r_{\mathrm{MT}})$, leading to a step of $\psi_+^{(\mathrm{L})}(\boldsymbol{r})$ at the surface of the muffin-tin sphere.

The Fourier coefficients of $\psi_+^{(\mathrm{L})}(\boldsymbol{r})$ can be easily calculated:

$$v(\boldsymbol{G}) = \frac{4\pi}{\Omega_0} c \left[ \frac{\Omega_0}{4\pi}\delta_{\boldsymbol{G},\mathbf{0}} - \int_0^{r_{\mathrm{MT}}} \mathrm{d}r \; w(r)\, j_0(|\boldsymbol{G}|r) \right] \tag{27}$$

with

$$w(r) = r^2 \left[ 1 - \frac{\psi_{\mathrm{sph}}(r)}{c} \right]. \tag{28}$$

$\Omega_0$ is the volume of the unit cell, and $j_0(x)$ means the spherical Bessel function of zeroth order. Due to the discontinuity of $\psi_+^{(\mathrm{L})}(\boldsymbol{r})$ for $|\boldsymbol{r}| = r_{\mathrm{MT}}$, $w(r)$ is not necessarily zero for the argument $r = r_{\mathrm{MT}}$.

Equation (27) teaches us that the sensitivity of the Fourier coefficients $v(\boldsymbol{G})$ with respect to (small) changes of the positron wave function will be determined by (i) the details of the change of $w(r)$ and (ii) the oscillatory behaviour of the Bessel function $j_0$. These oscillations increase with increasing $|\boldsymbol{G}|$ leading to a partial cancellation of the positive and negative parts of the integral in equation (27). Due to this fact, a change of $w(r)$ will influence the integral values and the Fourier coefficients of $\psi_+^{(\mathrm{L})}$. The greater the values of $|\boldsymbol{G}|$ are, the greater this influence will be. Therefore, we expect that the sensitivity of $v(\boldsymbol{G})$ with respect to $w(r)$ will be small for $\boldsymbol{G} = (000)$, moderate for reciprocal-lattice vectors $\boldsymbol{G} \neq (000)$ which lie near to the central BZ (i.e. for $\boldsymbol{G} = (110)$ and $\boldsymbol{G} = (111)$ for bcc and fcc structures, respectively), and might be large for Brillouin zones far away from the centre. Figure 3 illustrates this argumentation for lithium (for other metals, the situation is similar).

The above considerations are strongly confirmed by extensive numerical tests where we investigated the sensitivity $\Delta\rho_+$ (equation (6)) for the bcc metals Li, Na, K, Rb, Cs, and V and for the fcc metals Al, Cu, and Pd [24]. For these tests, we slightly changed the functions $\psi_{\mathrm{sph}}(r)$ (to give an impression of the strength of this change, we mention

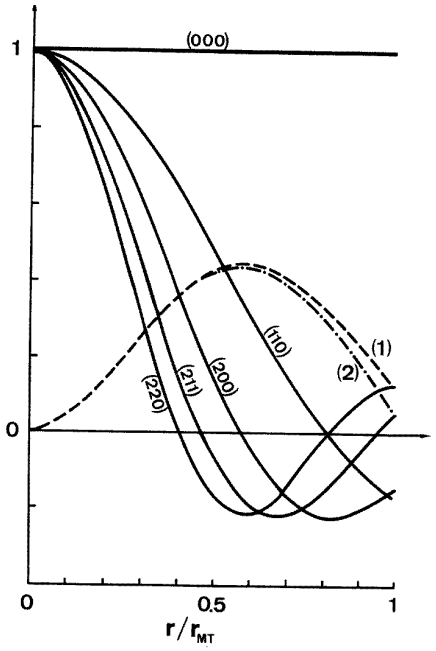


**Figure 3.** $w^{(1)}(r)$ and $w^{(2)}(r)$ as functions of $r/r_{\mathrm{MT}}$ inside the muffin-tin sphere for lithium are represented by broken and chain curves, respectively. The numbers (1) and (2) refer to two slightly different approximations to the positron wave functions as described in section 2.3 of this paper. The full curves refer to the Bessel functions of zeroth order $j_0(|\boldsymbol{G}|r)$ for the reciprocal-lattice vectors $\boldsymbol{G} = (000)$, (110), (200), (211) and (220).

here that the relative deviation between the original (curve (1)) and the changed (curve (2)) functions on the surface of the muffin-tin sphere was about 1.3% for all metals investigated). These relatively small deviations of $\psi_{\mathrm{sph}}(r)$ lead to significant changes of the corresponding functions $w(r)$ (equation (28)) as is demonstrated for lithium in figure 3.

For the bcc metals, we obtained the following values of $\Delta\rho_+(\boldsymbol{G})$: for the central momentum region ($\boldsymbol{G} = (000)$), we got $\Delta\rho_+$ between 0.03 and 0.07%, and for the nearest Umklapp regions (centred around $\boldsymbol{G} = (110)$ and equivalent vectors) we got $\Delta\rho_+$ between 1.3 and 3.0%. For $\boldsymbol{G} = (200)$, the values of $\Delta\rho_+$ dramatically increase—up to 14% for V or even 22% for Li. For the fcc metals (Al, Cu, and Pd), the situation is similar: small sensitivities for $\boldsymbol{G} = (000)$, moderate $\Delta\rho_+$-values for the (111) and (200) Umklapp regions, and extremely high values for the BZ with a greater distance to the centre: $\Delta\rho_+ > 80\%$ for $\boldsymbol{G} = (220)$.

## 3. Summary

In this paper, we have studied the influence of the approximations used in calculating the positron wave function on the electron–positron momentum densities. The two cases $\boldsymbol{G} = \boldsymbol{G}_{kj}$ (the leading term of the density describing the Fermi surface in the extended-zone scheme) and $\boldsymbol{G} \neq \boldsymbol{G}_{kj}$ (describing Umklapp components) were considered separately. Our theory, which explains numerical results obtained in [19–24], leads to the following conclusions.

(i) $\Delta\rho(\boldsymbol{G}_{\boldsymbol{k}j})$, describing changes of the leading component of the density, can be either greater or smaller than $\Delta\rho_+(\boldsymbol{0})$. Nevertheless, because $|\kappa(\boldsymbol{G}_{\boldsymbol{k}j})| \ll 1$ (see section 2.1) and $\Delta\rho_+(\boldsymbol{0}) \ll 1$, $\Delta\rho(\boldsymbol{G}_{\boldsymbol{k}j})$ is always very small.

(ii) For all *relevant* Umklapp components of the density, we have

$$\Delta\rho(\boldsymbol{k}+\boldsymbol{G}) < \Delta\rho_+(\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j}).$$

(iii) The Fourier coefficients of the positron wave function for $\boldsymbol{G}-\boldsymbol{G}_{\boldsymbol{k}j}$—as reciprocal-lattice vectors belonging to Brillouin zones which are near to the central region of the momentum space—are generally only weakly sensitive to the approximations used in calculating the positron wave function, i.e. the corresponding values of $\Delta\rho_+$ are small. Only if two approximations used in calculating $\psi_+$ are significantly different will higher values of $\Delta\rho_+$ occur [24].

(iv) For *relevant* Umklapp components, $y < 1$; and the higher the value of the Umklapp density, the smaller the value of $y$. In the extreme case of very high values of $|\alpha|$, $y$ and $\Delta\rho(\boldsymbol{k}+\boldsymbol{G})$ are close to zero.

These facts lead to the main conclusion of this paper, namely that in each metal there are some *stable* components of $\rho(\boldsymbol{k}+\boldsymbol{G})$, i.e. densities which are only weakly sensitive to the approximations used in the calculation of the positron wave function. This is remarkable because it is only these *stable* densities that have values which are high enough to be studied experimentally. This property of the MDAP is important for a reliable verification of various approaches used for obtaining a theoretical description of the electron–positron interaction (see the introduction).

Finally, we would like to point out that the theory presented here is even more general and could be applied for each case of arbitrary renormalized non-interacting quasiparticles in a periodic lattice potential. The only restrictions are an absence of nodes of the wave function of one of the quasiparticles and its constant value for $\boldsymbol{r} = 0$ (i.e. at the positions of the ions). In the case of non-interacting renormalized quasiparticles, one can consider such interacting particles where an interaction is included in their wave functions (such a treatment is applied in the LDA [6–8]). In this way, our theory can also be applied in the study of the influence of a correlation function $f(\boldsymbol{r})$ on the electron–positron densities within the LDA.

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