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UMKLAPP COMPONENTS OF THE POSITRON MOMENTUM DENSITY DEPENDING ON DIFFERENT MODELS FOR THE POSITRON WAVE FUNCTION

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In this paper, we present a numerical investigation about the question how sensitively Fourier coefficients of the positron wave function ψ_+ react to different (and not too strong) changes of ψ_+. In order to obtain general information about this problem, we studied this sensitivity for several bcc and fcc metals and for different models of the positron wave function. Summarizing our results, we can say that this sensitivity is generally small (or at least moderate) for Fourier coefficients belonging to reciprocal lattice vectors $\boldsymbol{G}$ which lie nearest to the centre of the momentum space. For the outer vectors $\boldsymbol{G}$, the amount of this sensitivity is strongly dependent on the crystal structure of the metal and on the special type of the change of the positron wave function.

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1. Introduction

We learned from our theoretical and numerical studies on the behaviour of the electron–positron momentum density $\rho(\boldsymbol{p})$ of non-interacting particles in a periodic lattice potential [1–3] that, in each metal, there are some umklapp components $\rho(\boldsymbol{p} = \boldsymbol{k} + \boldsymbol{G})$ which are only weakly sensitive on different approximations of the positron wave function ψ_+. Explicitly, our theory shows that, for all so-called *relevant* umklapp regions (i.e. umklapp components of remarkably high values) centred around certain reciprocal lattice vectors $\boldsymbol{G}$, the relative change of the electron–positron momentum density $\Delta\rho^{(\mathrm{A,B})}(\boldsymbol{k} + \boldsymbol{G})$ with respect to different

models (A) and (B) of ψ_+ (we call this the *sensitivity* of ρ) is always smaller than the corresponding sensitivity of some particular Fourier coefficients of ψ_+.

In this paper, we shall demonstrate that each metal has at least one (and often more than one) reciprocal lattice vector $\boldsymbol{G}$ with a relatively small corresponding value of $\Delta\tilde{\rho}^{(\mathrm{A,B})}(\boldsymbol{G})$. We show that this behaviour is quite general and occurs for different crystal structures and different models of ψ_+.

In Sec. 2 we give a short review of the basic formulae of our theory on this topic, which has been previously published in Refs. [1, 2]. The different models of ψ_+ which we used for our numerical tests are described in detail in Sec. 3. The results of this investigation for several bcc (Li, Na, K, Rb, Cs, V) and fcc metals (Al, Cu, Pd) are presented in Sec. 4.

2. Review of basic formulae

Following Ref. [4] within the independent particle model (IPM), the electron-positron momentum density (for a given electron band j) reads as

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

with

$$\alpha_{kj}(\boldsymbol{G}) = \sum_{\boldsymbol{H}\neq\boldsymbol{G}_{kj}} \frac{v(\boldsymbol{G}-\boldsymbol{H})u_{kj}(\boldsymbol{H})}{v(\boldsymbol{G}-\boldsymbol{G}_{kj})u_{kj}(\boldsymbol{G}_{kj})}. \tag{2}$$

In Eqs. (1) and (2), u_{kj} and v are the Fourier coefficients of the electron in the Bloch state kj and the thermalized positron wave function, respectively, and $\boldsymbol{G}_{kj}$ is the reciprocal lattice vector which describes the *leading coefficient* of the Fourier expansion of the electron wave function with the property $|u_{kj}(\boldsymbol{G}_{kj})| > |u_{kj}(\boldsymbol{H})|$. According to Refs. [1] and [2], the sensitivity of $\rho_j(\boldsymbol{k}+\boldsymbol{G})$ with respect to different approximations (A) and (B) of the positron wave function ψ_+ can be expressed by

$$\Delta\rho_j^{(\mathrm{A,B})}(\boldsymbol{k}+\boldsymbol{G}) = \left\{\left[\frac{v^{(m)}(\boldsymbol{G}-\boldsymbol{G}_{kj})}{v^{(l)}(\boldsymbol{G}-\boldsymbol{G}_{kj})}\right]\left[1+\kappa_{kj}^{(l,m)}(\boldsymbol{G})\right]\right\}^{2n} - 1, \tag{3}$$

where $n=+1$ for $\rho_j^{(m)} > \rho_j^{(l)}$ and $n=-1$ for $\rho_j^{(m)} < \rho_j^{(l)}$ and

$$v^{(m)} = \max\left\{|v^{(\mathrm{A})}|;|v^{(\mathrm{B})}|\right\} \quad \text{and} \quad v^{(l)} = \min\left\{|v^{(\mathrm{A})}|;|v^{(\mathrm{B})}|\right\} \tag{4}$$

with

$$\kappa_{kj}^{(l,m)}(\boldsymbol{G}) = \left[\alpha_{kj}^{(m)}(\boldsymbol{G}) - \alpha_{kj}^{(l)}(\boldsymbol{G})\right] / \left[1+\alpha_{kj}^{(l)}(\boldsymbol{G})\right]. \tag{5}$$

The corresponding sensitivity of the Fourier coefficients of the positron wave function belonging to the models (A) and (B) is defined by

$$\Delta\tilde{\rho}^{(\mathrm{A,B})}(\boldsymbol{G}) = \frac{\left(v^{(m)}(\boldsymbol{G})\right)^2 - \left(v^{(l)}(\boldsymbol{G})\right)^2}{\left(v^{(l)}(\boldsymbol{G})\right)^2}, \tag{6}$$

and the dependence between $\Delta\rho^{(\mathrm{A,B})}$ and $\Delta\tilde{\rho}^{(\mathrm{A,B})}$ is described by the positive ratio

$$y(\kappa_{kj}) = \Delta\rho_j^{(\mathrm{A,B})}(\boldsymbol{k}+\boldsymbol{G})/\Delta\tilde{\rho}^{(\mathrm{A,B})}(\boldsymbol{G}-\boldsymbol{G}_{kj}). \tag{7}$$

As a main result of our previous papers we got out that, for all relevant umklapp regions, $y(\kappa) < 1$, or, if the umklapp densities have a high value, $y(\kappa) \ll 1$, i.e. $\Delta\rho(\boldsymbol{k} + \boldsymbol{G})$ is very small (close to zero). This relation which has been both theoretically derived and checked by numerous numerical tests means that the sensitivity of the Fourier coefficients belonging to different models (A), (B) of ψ_+ is always an upper limit for the "true" sensitivity $\Delta\rho_j$ of the electron–positron momentum density.

3. Approximations of the positron wave function

In order to make this investigation practically useful, it is of great importance to choose models for the positron wave function $\psi_+(r)$ which are frequently used in realistic calculations of electron–positron annihilation rates.

As we extensively discussed in a previous paper on the role of approximations of ψ_+ in rate calculations [5], especially the authors who work with augmented plane wave (APW) or APW-related rate formulae frequently use approximations of ψ_+, where the spatial anisotropy of this function is partially or totally neglected. Nevertheless, it should be emphasized here that there are also rate formulae which are able to take into account the full anisotropy of ψ_+ without any approximations. We mention here the formula based on the Korringa–Kohn–Rostoker (KKR) method and a multiple-scattering formalism [6].

One of the most popular approximations of ψ_+ has been proposed by Loucks [7] and is of the *muffin-tin* type:

$$\psi_+^{(\mathrm{L})}(r) = \begin{cases} c & \text{for} \quad |r| > r_{\mathrm{MT}}\,, \\ \psi_{\mathrm{sph}}(r) & \text{for} \quad |r| \leq r_{\mathrm{MT}}\,, \end{cases} \tag{8}$$

where $\psi_{\mathrm{sph}}(r)$ is the spherical average of an APW positron wave function inside the muffin-tin sphere with radius r_{MT}. Outside this sphere, ψ_+ is approximated by the constant c. Due to this special procedure, c does generally not coincide with $\psi_{\mathrm{sph}}(r = r_{\mathrm{MT}})$ leading to a step of $\psi_+^{(\mathrm{L})}(r)$ at the surface of the muffin-tin sphere. As all positron wave functions used in our work, $\psi_+^{(\mathrm{L})}$ is normalized to the unit cell of the crystal lattice Ω_0. Obviously, $\psi_+^{(\mathrm{L})}$ does not at all take into account any spatial anisotropy of the "true" positron wave function.

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

$$v_+^{(\mathrm{L})}(\boldsymbol{G}) = \frac{4\pi}{\Omega} c \left[\frac{\Omega}{4\pi} \delta_{\boldsymbol{G},\mathbf{0}} - \int_0^{r_{\mathrm{MT}}} \mathrm{d}r\, w(\mathrm{r})\, j_0(Gr) \right] \tag{9}$$

with

$$w(r) = r^2 \left[1 - \frac{\psi_{\mathrm{sph}}(r)}{c} \right], \tag{10}$$

where $j_0(x)$ means the spherical Bessel function of zero-th order. Due to the discontinuity of $\psi_+^{(\mathrm{L})}(r)$ for $|r| = r_{\mathrm{MT}}$, $w(r_{\mathrm{MT}})$ is not necessarily zero.

If one decides to proceed from $\psi_+^{(\mathrm{L})}$ to a more realistic approximation of the positron wave function, the following typical "perturbations" of the approximation

according to Loucks will appear: There will be changes of ψ_+ *inside* the muffin-tin sphere, especially close to the muffin-tin radius r_{MT}. Such changes can be modeled by the definition of a "perturbed Loucks function" $\psi_+^{(Lp)}$ which is based on

$$\psi_{sph}^{(p)}(r) = \begin{cases} \psi_{sph}(r) & \text{for } r < r_0\,, \\ \psi_{sph}(r)\,[1+\gamma(r-r_0)/a] & \text{for } r \geq r_0, \end{cases} \tag{11}$$

with $r_0 < r_{MT}$ and a as the lattice constant of the metal. The strength of this perturbation can be controlled by the two parameters γ and r_0. The perturbed Fourier coefficients $v^{(Lp)}(\boldsymbol{G})$ and the corresponding function $w^{(p)}(r)$ are defined by Eqs. (9) and (10) with $\psi_{sph}^{(p)}(r)$ (Eq. (11)) instead of $\psi_{sph}(r)$. Additionally, a new (perturbed) normalization constant $c^{(p)}$ will also appear.

According to Eq. (9), one can generally expect that the sensitivity of $v_+^{(L)}(\boldsymbol{G})$ will increase with an increasing oscillatory behaviour of the Bessel function $j_0(Gr)$, which is strongly connected with the number and the position of the nodes of this function inside the muffin-tin sphere. Taking this into account, one expects very small changes in $v_+^{(L)}(\boldsymbol{G})$ for $\boldsymbol{G} = (000)$ (in this case, $j_0(Gr) = 1$), and moderate changes for the first non-zero reciprocal lattice vector ($\boldsymbol{G} = (110)$ or (111) for bcc and fcc structures, respectively). In both cases $j_0(Gr)$ has only one node inside the muffin-tin sphere close to r_{MT}. For $\boldsymbol{G} = (200)$, the Bessel function has also only one node inside the muffin-tin sphere, but, for the bcc case, this node lies significantly deeper inside the sphere than for the fcc case ($r_{node}/r_{MT} = 1/\sqrt{3}$ and $1/\sqrt{2}$ for bcc and fcc, respectively). Consequently, the changes in $v_+^{(L)}(\boldsymbol{G})$ for $\boldsymbol{G} = (200)$ are expected to be greater for the bcc than for the fcc structure. This expectation is strongly confirmed by our numerical tests which are discussed in the following section.

Anisotropy effects in the *interstitial region* (i.e. between the muffin-tin sphere and the boundaries of the Wigner–Seitz cell) are included in the approximation of ψ_+ proposed by Hubbard and Mijnarends [8]:

$$\psi_+^{(M)}(r) = \begin{cases} \psi_{sph}(r) & \text{for } |r| \leq r_{MT}\,, \\ \sum_{\boldsymbol{K}} b(\boldsymbol{K}) e^{i\boldsymbol{K}\cdot\boldsymbol{r}} & \text{for } |r| > r_{MT}\,, \end{cases} \tag{12}$$

what means that, outside the muffin-tin sphere, the wave function is described by a plane-wave expansion. The corresponding Fourier coefficients are given by the expression

$$v_+^{(M)}(\boldsymbol{G}) = \frac{4\pi}{\Omega}\left[\frac{\Omega}{4\pi} b(\boldsymbol{G}) - r_{MT}\sum_{\boldsymbol{K}} b(\boldsymbol{K})\chi(|\boldsymbol{K}-\boldsymbol{G}|r_{MT}) + \int_0^{r_{MT}} dr\, r^2\, \psi_{sph}(r) j_0(Gr)\right] \tag{13}$$

with $\chi(x) = j_1(x)/x$ and $j_1(x)$ as the spherical Bessel function of the first order.

So, we can resume as follows: The sensitivity values $\Delta\tilde{\rho}^{(L,Lp)}$ and $\Delta\tilde{\rho}^{(L,M)}$ (defined in Eq. (6)) give information how sensitive the Fourier coefficients of the positron wave function react to changes of ψ_+ inside and outside the muffin-tin region, respectively.

4. Numerical results and discussion

In this section, we show some numerical results on the sensitivity of the Fourier coefficients of ψ_+ according to Eq. (6) with respect to the different models $\psi_+^{(L)}$, $\psi_+^{(Lp)}$ and $\psi_+^{(M)}$ described in the previous section. In fact, we discuss the quantities $\Delta\tilde{\rho}^{(L;Lp)}(\boldsymbol{G})$ and $\Delta\tilde{\rho}^{(L;M)}(\boldsymbol{G})$ as functions of the reciprocal lattice vector $\boldsymbol{G}$ for several bcc and fcc metals. In our numerical work, we used three different sets of parameters r_0 and γ for $\psi_+^{(Lp)}$ (compare Eq. (11)), namely, for the bcc metals,

(Lp1): $r_0 = 0.3$; $\gamma = 0.05$,
(Lp2): $r_0 = 0.3$; $\gamma = 0.1$,
(Lp3): $r_0 = 0.15$; $\gamma = 0.05$,

and, for the fcc metals,

(Lp1): $r_0 = 0.22$; $\gamma = 0.05$,
(Lp2): $r_0 = 0.22$; $\gamma = 0.1$,
(Lp3): $r_0 = 0.11$; $\gamma = 0.05$ (all values of r_0 are in units of a).

The strength of the perturbation increases from (Lp1) to (Lp3) as it is illustrated by Fig. 1, where we show the unperturbed and perturbed functions $w(r)$ (see Eq. (10)) for bcc lithium.

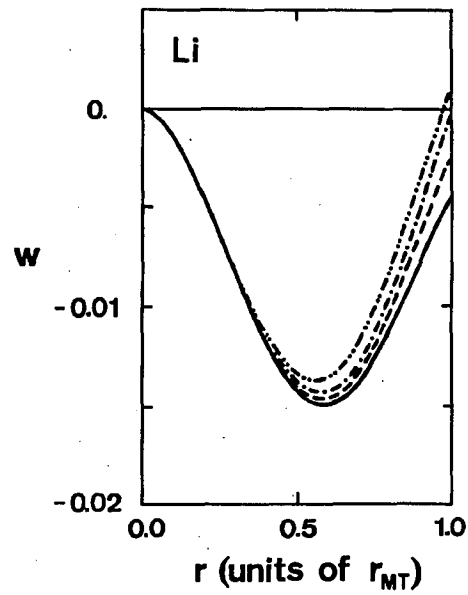

Fig. 1. Unperturbed and perturbed w and $w^{(P)}$ as functions of r in units of the muffin-tin radius for lithium. The full line means the unperturbed function according to Eq. (10). The perturbed functions $w^{(P)}$ (Eqs. (10) and (11)) which belong to the three different sets (Lp1), (Lp2), (Lp3) of parameters r_0 and γ as defined in Sec. 4 are represented by the dashed, dashed-dotted, and dashed-double-dotted line, respectively.

Tables I and II summarize our numerical results. We present values of $\Delta\tilde{\rho}^{(L;Lp)}(\boldsymbol{G})$ for the cases (Lp1), (Lp2), and (Lp3) and values of $\Delta\tilde{\rho}^{(L;M)}(\boldsymbol{G})$, both for the bcc metals Li, Na, K, Rb, Cs, and V and for the fcc metals Al, Cu, and Pd as well as for different reciprocal lattice vectors $\boldsymbol{G}$.

TABLE I

The sensitivity $\Delta\tilde{\rho}^{(A,B)}(\boldsymbol{G})$ (in %) for $\boldsymbol{G} = (110)$ and (111) (in units of $2\pi/a$), with respect to different approximations of the positron wave function. L — Loucks' approximation, Eq. (8); Lp1, Lp2, Lp3 — Loucks' approximation, perturbed in the way described in Secs. 3 and 4; M — approximation of Hubbard and Mijnarends, Eq. (12).

Metal	$\boldsymbol{G}$	$\lvert\Delta\tilde{\rho}^{(L,Lp1)}\rvert$	$\lvert\Delta\tilde{\rho}^{(L,Lp2)}\rvert$	$\lvert\Delta\tilde{\rho}^{(L,Lp3)}\rvert$	$\lvert\Delta\tilde{\rho}^{(L,M)}\rvert$
Li bcc	(110)	1.354	2.758	7.157	1.588
Na bcc	(110)	1.032	2.097	5.263	1.555
K bcc	(110)	0.804	1.630	3.938	1.619
Rb bcc	(110)	0.732	1.483	3.527	1.653
Cs bcc	(110)	0.658	1.332	3.103	1.699
V bcc	(110)	0.621	1.258	2.907	1.869
Al fcc	(111)	1.451	2.958	4.478	11.58
Cu fcc	(111)	1.389	2.829	4.249	10.53
Pd fcc	(111)	1.122	2.281	3.313	11.87

In Table I, we show results for the vectors $\boldsymbol{G}$ which lie nearest to the centre of the momentum space, namely $\boldsymbol{G} = (110)$ and $\boldsymbol{G} = (111)$ for the bcc and fcc metals, respectively (all $\boldsymbol{G}$ vectors are given in the units $2\pi/a$). It is evident from this table that, for all bcc metals investigated, the sensitivity of the Fourier coefficients of the positron wave function with respect to all models of ψ_+ which we discussed in Sec. 3 (Loucks, perturbed Loucks (Lp1), (Lp2), (Lp3) and Hubbard–Mijnarends) is very moderate. For $\Delta\tilde{\rho}^{(L,Lp1)}$), $\Delta\tilde{\rho}^{(L,Lp2)}$, and $\Delta\tilde{\rho}^{(L,M)}$, we observe very small sensitivity values between 0.6% up to about 2.8%. Only for the strongest perturbation of ψ_+ according to Loucks' formula, namely for $\Delta\tilde{\rho}^{(L,Lp3)}$, somewhat higher sensitivity values up to 7.2% appear. For the fcc metals investigated, the results for all three types of $\Delta\tilde{\rho}^{(L,Lp)}$ for $\boldsymbol{G} = (111)$ are quite similar to those for the bcc metals (values between $\approx 1.1\%$ to $\approx 4.5\%$). It is interesting that the sensitivity of ψ_+ with respect to changes outside the muffin-tin sphere, represented by $\Delta\tilde{\rho}^{(L,M)}$, is significantly stronger for fcc than for bcc metals: one observes sensitivity values of about 10–11% for our examples Al, Cu and Pd.

Table II contains our sensitivity results for the second-nearest reciprocal lattice vector $\boldsymbol{G} = (200)$. As an overall result for the bcc metals, we can say that all sensitivity values belonging to $\boldsymbol{G} = (200)$ are significantly higher than the corresponding $\Delta\tilde{\rho}$ values for $\boldsymbol{G} = (110)$ presented in Table I. With regard to the $\Delta\tilde{\rho}^{(L,Lp)}$ values for $\boldsymbol{G} = (200)$ for the fcc metals, the sensitivity is remarkably

TABLE II

The sensitivity $\Delta\tilde{\rho}^{(A,B)}(\boldsymbol{G})$ (in%) for $\boldsymbol{G} = (200)$ (in units of $2\pi/a$), with respect to different approximations of the positron wave function. The notation of this table is equal to that of Table I.

Metal	$\boldsymbol{G}$	$\lvert\Delta\tilde{\rho}^{(L,Lp1)}\rvert$	$\lvert\Delta\tilde{\rho}^{(L,Lp2)}\rvert$	$\lvert\Delta\tilde{\rho}^{(L,Lp3)}\rvert$	$\lvert\Delta\tilde{\rho}^{(L,M)}\rvert$
Li bcc	(200)	10.84	22.29	36.81	34.31
Na bcc	(200)	8.271	16.91	27.44	33.39
K bcc	(200)	7.084	14.44	23.05	39.22
Rb bcc	(200)	6.790	13.83	21.93	42.78
Cs bcc	(200)	6.558	13.35	21.00	48.44
V bcc	(200)	7.132	14.54	22.76	66.60
Al fcc	(200)	1.460	2.927	2.550	39.85
Cu fcc	(200)	1.366	2.739	2.403	34.58
Pd fcc	(200)	1.207	2.419	2.185	42.46

small, approximately equal or even smaller than the corresponding values for the nearest reciprocal lattice vector of Table I. However, for the sensitivity values $\Delta\tilde{\rho}^{(L,M)}$, the situation is quite clear: for $\boldsymbol{G} = (200)$, for all metals investigated, we observe a very high sensitivity of the Fourier coefficients of ψ_+ with respect to changes of ψ_+ in the interstitial region.

5. Summary and conclusions

This contribution is dedicated to a numerical study of the question, how sensitively the Fourier coefficients of a muffin-tin positron wave function ψ_+ react to changes of ψ_+ both inside and outside the muffin-tin sphere. For this purpose, we use several models of ψ_+ (Loucks' formula, some perturbed versions of Loucks' formula, the formula proposed by Hubbard and Mijnarends), and we investigate the sensitivity of the Fourier coefficients as defined in Eq. (6) with respect to these approximations of ψ_+ for several examples of bcc and fcc metals and for different reciprocal lattice vectors $\boldsymbol{G}$.

As a general result of our investigation we can say: For all Fourier coefficients belonging to the reciprocal lattice vector which lies nearest to the centre of the momentum space (i.e. $\boldsymbol{G} = (110)$ and (111) for the bcc and the fcc case, respectively), this sensitivity is small or at least of moderate extent (Table I). For the next lattice vector ($\boldsymbol{G} = (200)$ both for bcc and fcc), the situation is more complicated because the sensitivity behaviour is much more dependent on the structure of the metal and on the special type of change of ψ_+ (Table II). For all bcc metals investigated, we generally observe relatively strong sensitivities. For the fcc metals, however, the sensitivity is weak for changes of ψ_+ inside the muffin-tin sphere (modeled by the types L and Lp) and rather strong for changes outside the muffin-tin sphere (modeled by the types L and M).

Our numerical tests presented here agree with our statement in Refs. [1, 2] that, for all metals and for different (not too strong) changes of the positron

wave function, there exists at least one Fourier coefficient which is weakly or only moderately sensitive to such changes.

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