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ELECTRON–POSITRON ENHANCEMENT IN *d*-METALS DESCRIBED BY BLOCH-MODIFIED LADDER THEORY AND LOCAL DENSITY APPROXIMATION: A COMPARATIVE STUDY

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In this paper, we present a preliminary summary of our recent results on the enhancement of the electron–positron annihilation rate in *d*-band metals based on our recently published optimized quasi-free Bloch-modified ladder [QF-BML(opt.)] theory. This approach enables us to investigate the influence of the periodical lattice potential on the electron–positron annihilation in an approximative but nevertheless physically reasonable way. We used our theory for calculations of momentum-dependent enhancement factors belonging to electron states of different (*s*-, *p*-, *d*-) character in simple, transition and noble metals (Na, Cu, Pd, V). It is interesting to compare these new BML results with corresponding results obtained by the local density approximation (LDA) according to the work of Daniuk et al. We observe relatively strong differences between the BML and LDA enhancement factors for metals whose polarization process is dominated by *s* or *p* electrons. In such cases, we presume that the LDA approach has the tendency to overestimate the role of the more-localized *d* electrons in the polarization of the inhomogeneous electron gas. For transition metals whose physics is mainly determined by such *d* electrons, the discrepancies between BML and LDA enhancement results are significantly smaller.

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1. Introduction

In a series of papers [1–3], we investigated the behaviour of positrons propagating within an inhomogeneous electron gas. Since Kahana's famous paper on the electron–positron enhancement in the homogeneous electron gas [4], many authors successfully dealt with the behaviour of positrons in jellium. It is not necessary

to describe this development here because some very competent review papers on this subject have been recently published (see e.g. Ref. [5]). In fact, we can say that the enhancement problem for the homogeneous electron gas is more or less solved.

However, this is by no means the case for the problem of the enhancement of positrons within the inhomogeneous electron gas as, for example, in a real metal. For a theoretical description of the electron–positron interaction in solids, there exist two different concepts.

(i) The so-called Bloch-modified ladder (BML) theory is the application of the Kahana formalism to the inhomogeneous electron gas. During the last years, some efforts have been made for a physically realistic description of the electron and positron scattering states which appear in the ladder formalism (the Bethe–Goldstone equation) turning out that lattice effects with respect to both the interacting electron and positron Green's functions and the polarization of the electron gas due to the positron play an important role and must not be neglected [1–3, 6, 7]. Recently, we presented a new and improved version of our so-called "quasi-free" BML (QF-BML) approach [8] by optimizing the two parameters α_e and α_p which appear in our QF-BML formulae: this new version, called optimized quasi-free Bloch-modified ladder theory [QF-BML(opt.)] [3] is one of the starting points of the investigation presented here.

(ii) Another very effective and successful theoretical approach for the description of electron–positron enhancement effects in solids is based on the use of *local* state-dependent enhancement factors in the independent particle model (IPM) rate formula: therefore, this approach which goes back to a paper of Bonderup et al. [9] and has been further developed by Daniuk et al. [10] is called the local density approximation (LDA). A comprehensive summary about the success and the problems of this theory has been recently presented by Šob [11].

The aim of this work is a comparison of the momentum-dependent enhancement results obtained both by BML and LDA where we are especially interested in the question how *d*-bands in the neighbourhood of the Fermi energy may influence the enhancement. Therefore, after a short review of the theoretical background of this paper given in Secs. 2–4, we focus our attention to electron–positron interactions in noble and transition metals like copper, palladium and vanadium. Nevertheless, it is also very interesting to study the differences of LDA and BML results in simple (and very "jellium-like") metallic systems like sodium.

2. Basic theory

All theoretical investigations on the electron–positron behaviour in condensed matter are based on the formula for the momentum-dependent two-particle annihilation rate [12]:

$$R(\boldsymbol{p}+\boldsymbol{G}) = \frac{\lambda}{\Omega}(-\mathrm{i})^2 \int_{\Omega} \mathrm{d}^3x\,\mathrm{d}^3y\, \exp\left[-\mathrm{i}(\boldsymbol{p}+\boldsymbol{G})\cdot(\boldsymbol{x}-\boldsymbol{y})\right] G_{\mathrm{ep}}(\boldsymbol{x}t, \boldsymbol{x}t; \boldsymbol{y}t^+, \boldsymbol{y}t^+), \qquad (1)$$

where λ/Ω means the Sommerfeld rate. $\hbar(\boldsymbol{p}+\boldsymbol{G})$ is the photon-pair momentum which is, for practical reasons, defined by the sum of a vector $\boldsymbol{p}$ inside the first

Brillouin zone (BZ) and a reciprocal lattice vector $\boldsymbol{G}$. For $\boldsymbol{G} \neq \boldsymbol{0}$, the formula deals with high-momentum (umklapp) components of the electron–positron momentum density, whereas $\boldsymbol{G} = \boldsymbol{0}$ corresponds to the central momentum region. For this contribution, all calculations were performed for $\boldsymbol{G} = \boldsymbol{0}$. G_{ep} represents the zero-temperature electron–positron Green's function. Following Kahana [4], G_{ep} can be expanded in a series of so-called ladder diagrams

$$G_{\mathrm{ep}}(x, x'; y, y') = G_{\mathrm{e}}(x, y) G_{\mathrm{p}}(x', y') + \frac{\mathrm{i}}{\hbar} \int \mathrm{d}\xi \mathrm{d}\eta \, G_{\mathrm{e}}(x, \xi) G_{\mathrm{p}}(x', \eta) v_{\mathrm{ep}}(\xi, \eta) \times G_{\mathrm{ep}}(\xi, \eta; y, y') \tag{2}$$

($x \equiv \boldsymbol{x} t_x$ etc.) with G_{e} and G_{p} as the single-particle Green's functions of the electron and positron, respectively, which are based on the eigenfunctions φ and ψ of the single-particle Schrödinger equations

$$\left[-\frac{\hbar^2}{2m} \Delta + v_{\mathrm{c}}^{-}(r) + v_{\mathrm{xc}}^{-}(r) \right] \varphi_{n\boldsymbol{k}}(r) = \varepsilon_{n\boldsymbol{k}}^{-} \varphi_{n\boldsymbol{k}}(r), \tag{3}$$

$$\left[-\frac{\hbar^2}{2m} \Delta + v_{\mathrm{c}}^{+}(r) + v_{\mathrm{corr}}^{+-}(r) \right] \psi_{n\boldsymbol{k}}(r) = \varepsilon_{n\boldsymbol{k}}^{+} \psi_{n\boldsymbol{k}}(r). \tag{4}$$

In the above equations, $v_{\mathrm{c}}^{\pm}$ means the Coulomb potential energy of the particle due to the (rigid) lattice of the atomic ions and the Hartree potential. v_{xc}^{-} represents the LDA of the exchange and the (static) correlation of the electron with the other electrons. The term v_{corr}^{+-} in the positron equation represents the correlation interaction of the positron with the electrons. This correlation term is neglected in many theoretical investigations and also in the work presented here. But it should be emphasized that this neglect might not be justified in each case. Namely, as we learned from a recent paper of Daniuk, Šob and Rubaszek [13], this correlation effect on the positron state may considerably influence the annihilation probability, especially if the core annihilation is concerned. Nevertheless, the influence of the direct electron–positron correlation is normally much more important than this self-energy effect.

Taking into account only the first term of the ladder expansion (2) (the term of zeroth order with respect to a direct e^{+}–e^{-} interaction), we get

$$G_{\mathrm{ep}}^{(0)}(x, x'; y, y') = G_{\mathrm{e}}(x, y) G_{\mathrm{p}}(x', y').$$

Inserting this into the rate formula (1), one gets the well-known expression

$$R^{(0)}(\boldsymbol{p} + \boldsymbol{G}) = \frac{\lambda}{\Omega} \sum_{n} \Theta(\varepsilon_{\mathrm{F}} - \varepsilon_{n\boldsymbol{p}}) \left| \int_{\Omega} \mathrm{d}^3 r \, \exp\left[-\mathrm{i}(\boldsymbol{p} + \boldsymbol{G}) \cdot \boldsymbol{r} \right] \varphi_{n\boldsymbol{p}}(r) \psi_{+}(r) \right|^2 \tag{5}$$

with $\psi_{+} \equiv \psi_{10}$ as the bottom state of the positron.

Now, for a progress of the theoretical description of R, one may try to evaluate (at least approximately) the further terms of the integral equation (2) as we do it in our BML work, or one may include this effect of the direct e^{-}–e^{+} correlations by the insertion of an enhancement factor $\gamma_{n\boldsymbol{p}}[r_{\mathrm{s}}(r)]$ which is a function of the local electron density at a given point r: this procedure leads directly to the LDA rate formula

$$R^{\mathrm{LDA}}(p+G) = \frac{\lambda}{\Omega}\sum_n \Theta(\varepsilon_{\mathrm{F}} - \varepsilon_{np}) \times \left| \int_\Omega \mathrm{d}^3 r \exp\left[-\mathrm{i}(p+G)\cdot r\right] \sqrt{\gamma_{np}(r)}\, \varphi_{np}(r)\psi_+(r)\right|^2. \tag{6}$$

For the sake of brevity, we do not want to discuss in detail the different forms of γ which have been proposed by many authors during the last years. For our comparative LDA calculations, we always used the formulation of Daniuk et al. [10, 13] where γ is taken from the enhancement theory of the homogeneous electron gas

$$\gamma_{nk} = E_{\mathrm{hom}}\left[r_{\mathrm{s}}(r), X_{nk}\right]$$

with $X_{nk} = \sqrt{\varepsilon^-_{nk}/\varepsilon_{\mathrm{F}}}$ where ε^-_{nk} and ε_{F} mean the energy of the electronic state (nk) and the Fermi energy, respectively. This energy-dependent enhancement for individual states was proposed first by Šob [14, 15] and independently by Mijnarends and Singru [16].

3. The Bloch-modified ladder theory

The mathematical implications and problems combined with the application of Kahana's theory to the inhomogeneous electron gas (Carbotte [12] and Carbotte and Salvadori [17]) have been recently discussed by several authors [1–3, 6, 7]. We shall give here only a very short review of this topic.

The BML rate formula reads

$$R^{\mathrm{BML}}(p+G) = 2\frac{\lambda}{\Omega}\sum_n \Theta(\varepsilon_{\mathrm{F}} - \varepsilon_{np}) \left\{ \sum_K a_{np}(K) b_0(G-K) + \frac{1}{\Omega^2}\sum_i \sum_k \Theta(\varepsilon_{ik} - \varepsilon_{\mathrm{F}}) \sum_j \left(\epsilon_{np} - \varepsilon_{ik} + \varepsilon_0^+ - \varepsilon_{jq}^+\right)^{-1} \chi_{ij}^{\mathrm{BML}}(k) \times \sum_{G_1}\sum_{G_2} v^{\mathrm{ep}}_{G_1,G_2}(q) \left[\sum_{K_2} a_{np}(K_2) a_{ik}(K_2 - G_1 + L)\right] \times \left[\sum_{K_3} b_0(K_3) b_{jq}(K_3 + G_2)\right] \right\}^2. \tag{7}$$

and contains the *Bloch-modified Bethe–Goldstone amplitude* χ^{BML}

$$\chi^{\mathrm{BML}}_{i,j}(k) = \sum_{K_1} a_{ik}(K_1) b_{jq}(G - K_1 + L) + \frac{1}{\Omega^2}\sum_s \sum_{k'} \Theta(\varepsilon_{sk'} - \varepsilon_{\mathrm{F}}) \times \sum_t \left(\varepsilon_{np} - \varepsilon_{sk'} + \varepsilon_0^+ - \varepsilon_{tq'}^+\right)^{-1} \chi^{\mathrm{BML}}_{s,t}(k') \sum_{G',G''} v^{\mathrm{ep}}_{G',G''}(q'') \times \left[\sum_{K_2} a_{ik}(K_2) a_{sk'}(K_2 - G' + L'')\right] \times \left[\sum_{K_3} b_{jq}(K_3) b_{tq'}(K_3 + G'' - L + L' - L'')\right]. \tag{8}$$

In Eqs. (7) and (8), the a_{np} (ε_{np}) and b_0 (ε_0^+) mean the Fourier coefficients (energies) of the *occupied* electron and positron Bloch states. All other Fourier coefficients and eigenenergies belong to the *non-occupied* region. The reciprocal lattice vectors $\boldsymbol{L}$, $\boldsymbol{L}'$, $\boldsymbol{L}''$ etc. are defined by $\boldsymbol{q} = \boldsymbol{p} - \boldsymbol{k} - \boldsymbol{L} \in$ 1st Brillouin zone etc., and $v^{\mathrm{ep}}_{\boldsymbol{G}_1,\boldsymbol{G}_2}(\boldsymbol{q})$ represents the static approximation of the matrix of the effective electron–positron potential.

An important role in our theoretical calculations is played by an approximation of the above formulae which was first presented by Sormann and Puff [8]. This approach simplifies the mathematical structure of the *non-occupied* electron and positron states occurring in Eqs. (7) and (8). It employs the Sommerfeld-like approximations

$$\varepsilon_{i\boldsymbol{k}} \approx \varepsilon_{10} + \alpha_{\mathrm{e}}|\boldsymbol{k}+\boldsymbol{K}_i|^2, \qquad a_{i\boldsymbol{k}}(\boldsymbol{K}) \approx \delta_{\boldsymbol{K},\boldsymbol{K}_i},$$

$$\varepsilon^+_{j\boldsymbol{q}} \approx \varepsilon_0^+ + \alpha_{\mathrm{p}}|\boldsymbol{q}+\boldsymbol{K}_j|^2, \qquad b_{j\boldsymbol{q}}(\boldsymbol{K}) \approx \delta_{\boldsymbol{K},\boldsymbol{K}_j}, \tag{9}$$

where ε_{10} and ε_0^+ mean the electron and positron bottom energies, respectively. Additionally, the electron–positron interaction matrix is simply approximated by

$$v^{\mathrm{ep}}_{\boldsymbol{G}_1,\boldsymbol{G}_2}(\boldsymbol{q}) \approx v^{\mathrm{ep}}(|\boldsymbol{q}+\boldsymbol{G}_1|; N_{\mathrm{eff}})\,\delta_{\boldsymbol{G}_1,\boldsymbol{G}_2}.$$

The insertion of these approximations into Eqs. (5) and (6) leads to the *quasi-free* (QF) BML formula

$$R^{\mathrm{QF-BML}}(\boldsymbol{p}+\boldsymbol{G}) = 2\frac{\lambda}{\Omega}\sum_n \Theta(\varepsilon_{\mathrm{F}}-\varepsilon_{np})\left\{\sum_{\boldsymbol{K}_1} a_{np}(\boldsymbol{K}_1)b_0(\boldsymbol{G}-\boldsymbol{K}_1)\right.$$
$$\left.\times\left[1-\frac{1}{\Omega}\sum_{\boldsymbol{k}}\Theta(k_0-k_{\mathrm{F}})\,v^{\mathrm{ep}}(|\boldsymbol{p}-\boldsymbol{k}+\boldsymbol{K}_1)|; N_{\mathrm{eff}})\,\chi^{\mathrm{QF-BML}}_{\boldsymbol{p};\boldsymbol{G}}(\boldsymbol{k})\right]\right\}^2, \tag{10}$$

with $k_0 = [(\varepsilon_{\mathrm{F}}-\varepsilon_{10})/\alpha_{\mathrm{e}}]^{1/2}$ and the corresponding Bethe–Goldstone equation

$$\chi^{\mathrm{QF-BML}}_{\boldsymbol{p};\boldsymbol{G}}(\boldsymbol{k}) = \left(\varepsilon_{np}-\varepsilon_{10}-\alpha_{\mathrm{e}}k^2-\alpha_{\mathrm{p}}|\boldsymbol{p}+\boldsymbol{G}-\boldsymbol{k}|^2\right)^{-1}$$
$$\times\left\{1+\frac{1}{\Omega}\sum_{\boldsymbol{k}'}\Theta(k'-k_0)\,v^{\mathrm{ep}}(|\boldsymbol{k}-\boldsymbol{k}'|; N_{\mathrm{eff}})\,\chi^{\mathrm{QF-BML}}_{\boldsymbol{p};\boldsymbol{G}}(\boldsymbol{k}')\right\}. \tag{11}$$

Equations (10) and (11) contain the parameters α_{e} and α_{p}. Recently, we presented an optimization scheme for these parameters by comparing the BML and QF-BML rates [Eqs. (7), (8) and (10), (11), respectively] belonging to the first two terms of the ladder expansion (2). This procedure whose details are described in Ref. [3] is called the α-optimized quasi-free Bloch-modified ladder approach [QF-BML(opt.)] and enables us to describe the lattice effects of the electron–positron annihilation process in the inhomogeneous electron gas approximately but much more realistically than in all other theoretical approaches.

4. The effective electron–positron interaction

All our present work on positron enhancement in real metals is based on the random phase approximation (RPA) for the effective $e^- - e^+$ interaction potential. This procedure which ignores the existence of much better approximations of this potential [18–20] requires some justification. The reason is that, at the present stage of our work, we are especially interested in comparisons between the BML and LDA enhancement factors, and we found out that the relations between the results of these two approaches do not significantly depend on the detailed form of the interaction potential used. On the other side, the use of RPA considerably simplifies our calculations.

Therefore, in all our QF-BML(opt.) calculations presented here, we used the simple approximation

$$v^{\mathrm{ep}}(q; N_{\mathrm{eff}}) \approx -v^{\mathrm{RPA}}(q; N_{\mathrm{eff}}), \tag{12}$$

where N_{eff} is determined in the way described in Sec. 5.

However, and this is the main progress of our new calculations, in order to obtain the optimized (state-dependent) values for $\alpha_{\mathrm{e}}(np)$ and $\alpha_{\mathrm{p}}(np)$, we describe the electron–positron interaction potential as the complete potential *matrix* instead of a simple potential *function* [2]. This means that the optimized α_{e} and α_{p} reflect at least approximately all lattice effects which influence the electron–positron enhancement: the lattice effects arising from the particle propagators within the terms of the ladder expansion and also the lattice effects of the interaction potential.

5. Results and discussion

In this section, we present results of our recent investigations for the simple metal sodium, the noble metal copper and two transition metals palladium and vanadium. The choice of these metals is by no means arbitrary but is motivated by the very different electron band structure of these metals in the neighbourhood of the Fermi surface. In the case of Na, the $3s$ valence electron is very "free-electron"-like, and both the polarization and the enhancement behaviour should show only very small lattice effects. This is also — at least to some extent — the case of Cu whose valence band has a significant s/p character close to the Fermi energy, despite the fact that the $3d$ bands lying somewhat below ε_{F} might play a certain role in the polarization and enhancement process. Nevertheless, one may expect that the investigated lattice effects for Cu are rather small, too. This is certainly no more the case of Pd and V whose valence bands are strongly hybridized with d-bands lying tightly below or even partly above the Fermi energy. This fact should lead to very strong lattice effects both for the polarization and for the enhancement. As a first step of our calculations, we had to determine reasonable values of the effective number N_{eff} of interacting electrons per unit cell which is used in our QF-BML formulae. These values were obtained by a comparison of LDA results and results of the homogeneous electron theory of the enhancement at the center of the first BZ. In this way, we obtained the following values of N_{eff}: 1.22 for Na, 3.43 for Cu, 4.31 for Pd, and 3.82 for V.

The behaviour of the RPA interaction potentials for the four metals investigated is demonstrated in Figs. 1a–d where we show calculated diagonal elements of the potential matrices along the [110] direction in Na and V and along the [111] direction in Cu and Pd. For comparison, the diagrams also contain the homogeneous RPA functions for the N_{eff} values given above. These interesting results confirm at least partly our expectations: for Na (Fig. 1a), the deviations between v^{ep} for the inhomogeneous and homogeneous case are very small. It is interesting that the inhomogeneous potential almost perfectly coincides with the homogeneous result for $N_{\text{eff}} = 1$ which means that the lattice effects of the polarization are more or less negligible, and the value of $N_{\text{eff}} = 1.22$ extracted from LDA enhancement calculations is obviously too large! This is also the case for Cu (Fig. 1b) where the lattice effects of the polarization are much greater than for Na and the effective number of electrons engaged in the polarization process is significantly smaller than it is expected by the LDA results.

For two transition metals investigated, one observes the inverse effect: the LDA-predicted values of N_{eff} are too small and lead to significantly stronger potentials than the potentials obtained by the theory of the inhomogeneous electron gas: this effect can be explained by the dominant role of the *d* electrons in these metals for the polarization process and their high density-of-states (DOS) in the region around the Fermi energy. If one compares the electron band structures of Pd and V, it is also understandable that this "enhancement of N_{eff}" by lattice effects is significantly smaller for Pd (Fig. 1c) than for V (Fig. 1d).

Another important point are the non-diagonal elements of the polarization matrices. We see from the corresponding formula [2] that the strength of these elements gives some information about the local effects of the particle–particle interaction in the electron gas. For the sake of brevity, we do not present our final results on this topic which show that there are very small local effects for metals whose polarization is dominated by *s/p* electrons (Na and Cu) and that there are strong local effects for Pd and V where *d* electrons play the major role in the polarization.

Some of our results on momentum-dependent enhancement factors for different valence bands in Na, Cu, Pd and V are shown in Figs. 2a–d. As a general remark on our enhancement study we can say that we principally understand the physics behind the results but we are far away to be able to present an explanation of all the details. Much more efforts will be necessary to obtain a fully satisfying understanding of the enhancement behaviour of positrons in real metals.

Each of Figs. 2a–d contains three curves: the LDA enhancement curve (full line), an enhancement curve obtained by our QF-BML(opt.) theory including a non-local electron–positron potential function according to the theory of the homogeneous electron gas (curve with triangles). These two curves show how the enhancement is influenced by lattice effects within the electron and positron propagators of the ladder expansion which are not explicitly taken into account by the LDA approach. Some of these results have already been presented in Fig. 2 of Ref. [3]. The full lines with squares in Figs. 2a–d show the main results of the present contribution, namely our enhancement curves including the lattice ef-

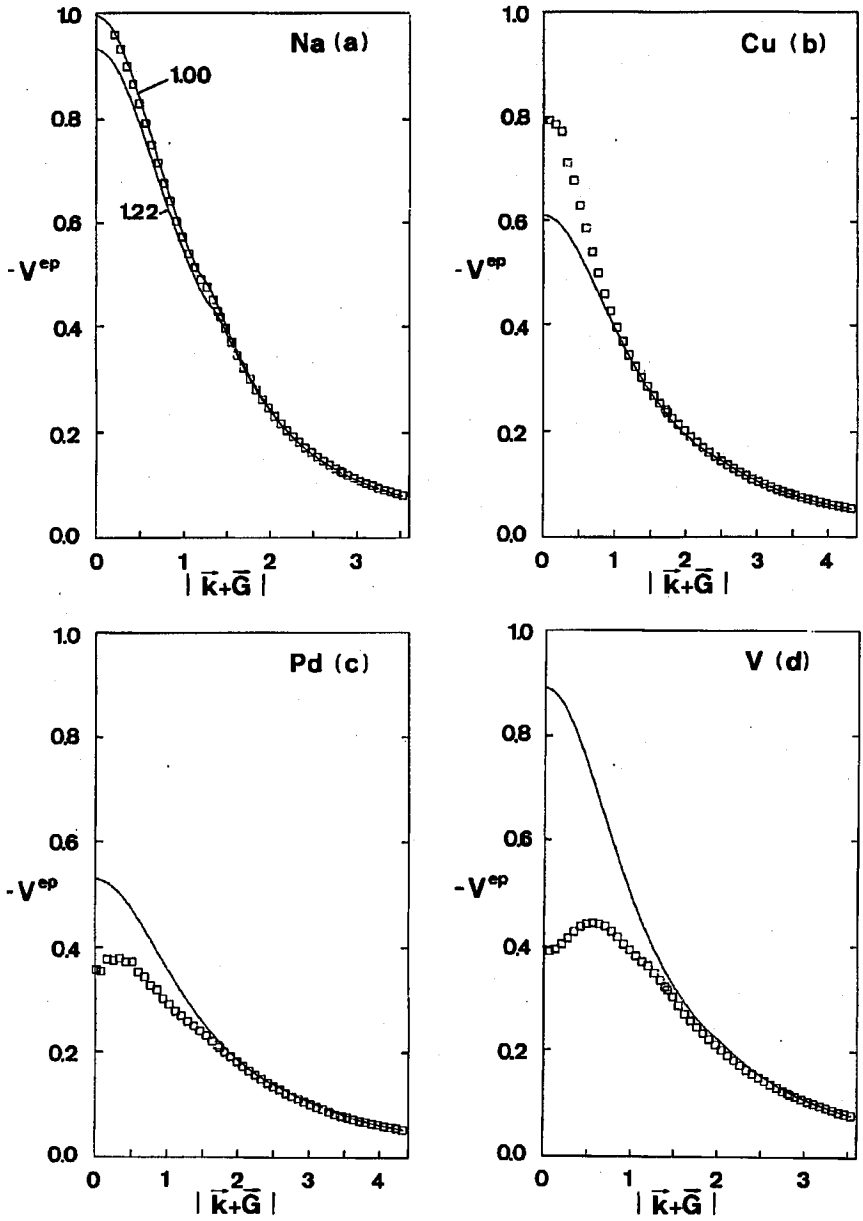

Fig. 1. Effective interaction potentials v^{ep} (in arbitrary units) in k space. The squares indicate the diagonal elements $v^{ep}_{G,G}(k)$ for $k \in$ 1st BZ and G are the reciprocal lattice vectors which lie closest to the centre of the first BZ. The full lines represent homogeneous RPA functions for (a) sodium ($N_{eff} = 1.00$ and 1.22), (b) copper ($N_{eff} = 3.43$), (c) palladium ($N_{eff} = 4.31$), and (d) vanadium ($N_{eff} = 3.82$). The momenta are in units of $2\pi/a$ where a is the lattice constant.

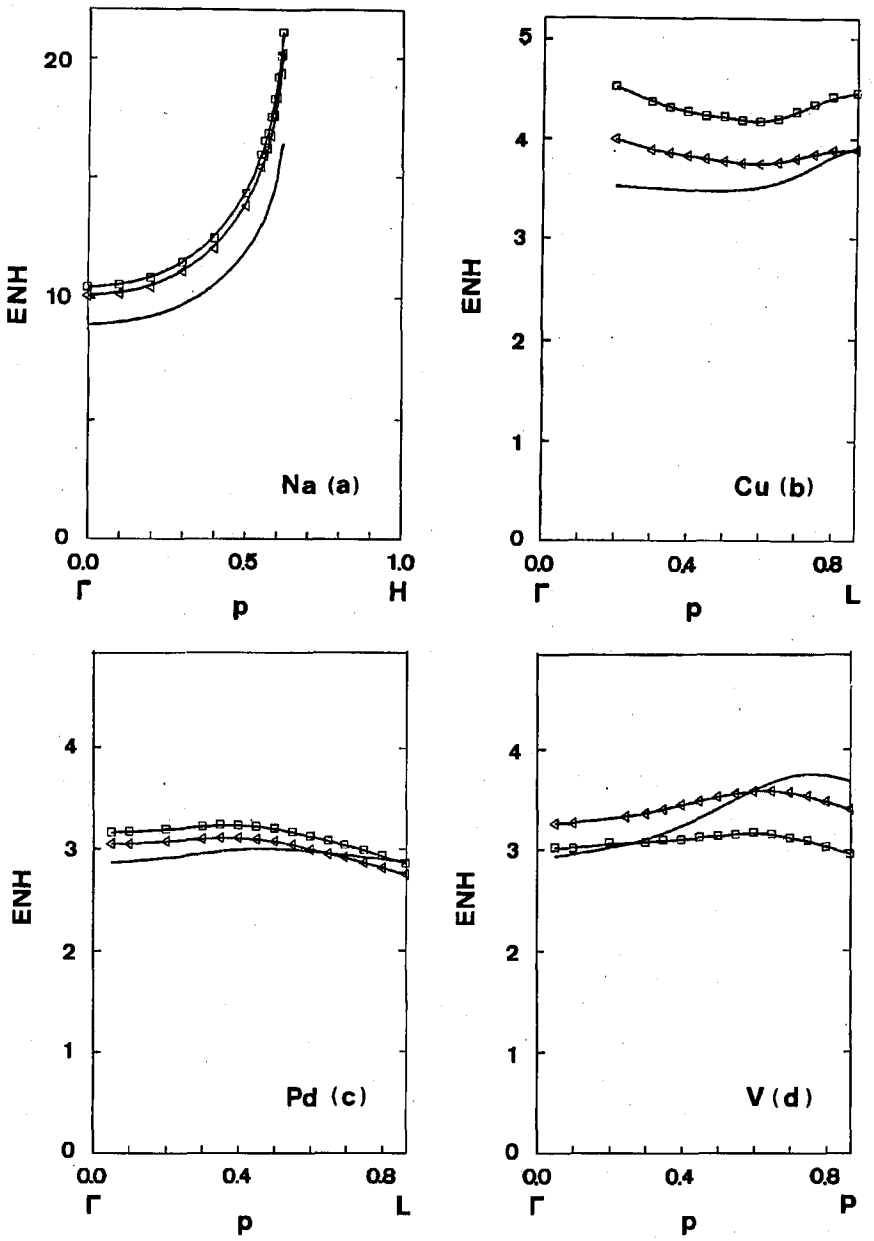

Fig. 2. State-dependent enhancement in simple, noble and transition metals as a function of the annihilation momentum p (given in units $2\pi/a$ with a as the lattice constant). Full curves: LDA; curves including triangles: QF-BML(opt.) including a non-local electron–positron potential function; curves including squares: QF-BML(opt.) including an electron–positron potential matrix with local effects. (a) Na, [100] direction, valence band, (b) Cu, [100], 6th valence band, (c) Pd, [111], 1st valence band, (d) V, [100], 1st valence band.

fects both from the electron and positron propagators and the electron–positron interaction potential. These results reflect more or less the results of Figs. 1a–d.

For Na (Fig. 2a), the enhancement curves belonging to the results of the QF-BML(opt.) approach with and without the influence of the lattice on the polarization are very similar due to the fact that these lattice effects are rather small. Nevertheless, both curves lie significantly above the LDA result, indicating relatively large lattice effects within the e^- and e^+ propagators. For Cu (Fig. 2b), the polarization is mainly determined by s/p electrons of the $4s$ valence band. The small DOS of these electrons close to ε_F leads to a significant increase in the strength of the effective interaction potential and, consequently, to an increase in the enhancement factors compared to the LDA results where the role of the copper $3d$ bands is obviously overestimated. This effect is especially large for enhancement curves belonging to occupied electron bands close to ε_F.

As far as the transition metals Pd and V are concerned, the situation is quite contrary: the polarization process is dominated by the d electrons of these metals with their relatively high DOS close to ε_F: therefore, the inclusion of lattice effects on the polarization into the enhancement theory causes a more or less strong reduction of the enhancement factors. We observe this behaviour very distinctly in the case of V (Fig. 2d) where the corresponding QF-BML(opt.) enhancement curves lie even below the LDA results. For Pd (Fig. 2c), these lattice effects with respect to the polarization are very small, much smaller than we would expect it from the behaviour of the interaction potential (compare Fig. 1c). In fact, for this material, the differences between the enhancement results belonging to BML and LDA are small for each occupied electron band and for each direction in the momentum space. At present, we have no convincing explanation for this rather surprising behaviour.

6. Conclusions

Our theoretical results on enhancement factors in simple, noble and transition metals and the comparison with LDA results clearly indicate that for a proper description of the electron–positron annihilation process in real (non jellium-like) metallic systems, an adequate theoretical consideration of the lattice effects of both the electron and positron scattering states and the effective interaction potential is necessary. Our comparison with LDA enhancement results shows that this approach has the tendency to overestimate the role of the d electrons for the polarization of the inhomogeneous electron gas. Therefore, in all metals where the polarization is dominated by s or p electron states (alkalis, copper), the LDA enhancement seems to be too small, whereas for metals with a high density of d states close to ε_F, the LDA approach is much more reliable. Consequently, in transition metals with their strong dominance of d electrons close to the Fermi surface, the agreement between LDA and our new BML approach is not bad (V) or even surprisingly satisfying (Pd). However, in metals whose scattering physics is dominated by s or p electrons (Na, Cu), the discrepancies between the LDA and BML results are considerably large.

Acknowledgments

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