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Mass enhancement factor for Pd and Pt

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Abstract. We report calculations of the mass enhancement factors for Pd and Pt by comparing the physical quantities using the interpolation scheme band structure, with the corresponding experimental data. Our results are compared with other theoretical calculations.

Keywords. Band structure; Fermi surface; effective mass.

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1. Introduction

In earlier papers we had reported calculations of the band structure and Fermi surface (FS) for Pd and Pt using the interpolation scheme where the parameters were chosen to fit the optical data as well as the FS extremal areas as measured by the dHvA experiments (Bordoloi and Auluck 1983a). It was shown that good agreement could be achieved if we define it in terms of a shift in Fermi level ΔE_F so that the calculated extremal area can be made to match with the experimental area. We find that extreme $\Delta E_F = 0{\cdot}0016$ Ry for Pt and 0·0022 Ry for Pd. We had also shown earlier that the calculated energy gaps at symmetry points (Bordoloi and Auluck 1983b) and $\varepsilon_2(w)$ (Bordoloi and Auluck 1988) were in good agreement with the experimental data.

In view of the success of our band structure in explaining the FS topology and the optical data, it would be interesting to calculate the dynamic properties of quasi-particles i.e. electron velocities $|\mathbf{v}_k^0|$, band masses m_b and density of states at the Fermi level $N(E_F)$. Comparison of these with the appropriate experimentally measured quantities yields three kinds of the enhancement factor. Our purpose here is to compare our calculated enhancement factor with other calculations and to see whether the enhancement factor obtained by the three different comparisons is consistent with each other.

Smith (1974) calculated the band structure of Pd and Pt using the combined interpolation scheme with the parameters chosen to fit the photoemission data obtained by him. Needless to say the agreement between this set of parameters and the experimental FS was rather poor (Bordoloi 1982). Hence the parameters were adjusted to obtain a good representation for the FS topology without destroying the agreement with optical data. This is referred to as our model, details of which are given elsewhere (Bordoloi 1982). Our model is so as to give a good agreement with optical data and FS geometry. We note in passing that with the interpolation scheme, which has numerous

parameters, this could be achieved whereas with *ab initio* band structure this is not possible (Jepsen *et al* 1981).

In this paper, we report calculations of $|\mathbf{v}_{\mathbf{k}}^0|$, m_b and $N(E_F)$ for Pd and Pt. We compare our calculations with some other more accurate *ab initio* calculations so that we can compare the enhancement factors obtained by using different band structures.

In § 2 a brief review of the interpolation scheme is presented. The details of the parameters were given earlier (Bordoloi and Auluck 1983a, b). In § 3 we mention how the various electronic properties are modified by the many body interactions. Calculations of $N(E_F)$ m_b, and $|\mathbf{v}_{\mathbf{k}}^0|$ are reported in §§ 4, 5 and 6 respectively.

2. Interpolation scheme

The combined interpolation scheme was originally devised by Hodges *et al* (1966) and Mueller (1967). We have used a variant of the original scheme (Smith and Mattheiss 1974). Here the *d*-electrons are represented in the tight-binding representation and the *s*-electrons by rapidly converging orthogonalized plane waves (OPW). The Bloch function is written as

$$\psi_{\mathbf{k}}(\mathbf{r}) = \sum_m \alpha_m |\phi_{\mathbf{k}m}\rangle + \sum_{\mathbf{G}} \alpha_{\mathbf{KG}} |\phi_{\mathbf{KG}}\rangle \tag{1}$$

where $|\phi_{\mathbf{k}m}\rangle$ is the usual light-binding wave function and $|\phi_{\mathbf{KG}}\rangle$ are the OPWs. In the original work only 4 OPWs were taken and since m has 5 values for the *d*-electrons, this gives a total of 9 unknown α's. The energy eigenvalues are given by the solution of the secular equation

$$\det |\langle \mathbf{k}\mu | H - E | \mathbf{k}\mu \rangle| = 0, \tag{2}$$

where we have written $|\mathbf{k}\mu\rangle$ for the ϕ's. Since there are 9 basis functions, this scalar equation is a 9×9 matrix. The matrix elements (equation (2)) have the form

$$H = \begin{vmatrix} H_{cc} & H_{cd} \\ H_{dc} & H_{dd} \end{vmatrix}, \tag{3}$$

where H_{cc} is a 4×4 matrix block arising from the OPW-OPW matrix elements. These are given by

$$\langle \phi_{\mathbf{KG}} | H | \phi_{\mathbf{KG}'} \rangle = \alpha q^2 \delta_{\mathbf{GG}'} + V_{\mathbf{GG}'} + S j_2(qR) j_2(q'R) P_2(\hat{q}\cdot\hat{q}'), \tag{4}$$

where $\mathbf{q} = \mathbf{k} + \mathbf{G}\cdot\alpha$, $V_{\mathbf{GG}'}$, δ and R are regarded as variable parameters. The H_{dd} is a 5×5 matrix block arising from the $d-d$ matrix elements and this is written in terms of variable parameters $E_0, \Delta, A_1, A_2, A_3, A_4, A_5$ and A_6 (Fletcher and Wohlfarth 1951 and Fletcher 1952; Slater and Köster 1954). The hybridization block H_{cd} is a 4×5 matrix block consisting of matrix elements between OPW and tight-binding functions. It is parametrized using

$$\langle \phi_{\mathbf{k}m} | H | \mathbf{k} \rangle = C_2 g(\mathbf{k}) Y_2^m(\hat{k}),$$

data. The enhancement factor is

$$1 + \lambda_\gamma = N_\gamma(E_F)/N(E_F). \tag{9}$$

This enhancement factor is of course a constant for a particular metal. λ_γ is the value of $\lambda_{\mathbf{k}}$ averaged over the entire FS.

Different band structures would give different values of $|\mathbf{v}_{\mathbf{k}}^0|$, m_b and $N(E_F)$ because they do not explicitly include the interactions. It is therefore obvious that the values of the λ's will depend on the band structure used. Hence there is some arbitrariness in the values of λ's. This should be noted when compared with other calculations. Also one can perform *ab initio* calculations of the enhancement factor by implicitly considering electron-electron and electron-phonon interactions. In Pd and Pt one has also to include spin fluctuations. Since these calculations are very involved and have not been done so far, we adopt the empirical approach in the present study.

We have calculated $\lambda_{\mathbf{k}}$, λ_c and λ_γ for both Pd and Pt using our model. We would like to state that the parameters of the interpolation scheme are different for Pd and Pt. Once the parameters are fixed (as in our model) $\lambda_{\mathbf{k}}$, λ_c and λ_γ are calculated with no more adjustment of the parameters. Results of such calculations are reported here.

4. λ using specific heat data

The linear specific heat coefficient γ has been measured by numerous workers (for a survey see Bordoloi 1982). We have used the latest value of γ which is the most accurate one obtained from very pure samples. We have evaluated $N(E_F)$ by first calculating $N(E)$ obtained by using the special directions method (Prasad and Bansil 1980) for the Brillouin zone integration. E_F was fixed by demanding that the integral of $N(E)$ gives the correct electrons/atom. Since E_F was on a rapidly changing $N(E)$, a small variation in E_F could give a large variation in $N(E_F)$ and hence λ. To obtain an accurate value for $N(E_F)$ we have to slice the Fermi surface.

The values of $(1 + \lambda_\gamma)$ obtained by different workers are given in table 1 along with our values. Our values (1·36 for Pd and 1·22 for Pt) are significantly lower than the values of 1·6–1·7 for Pd and 1·5–1·6 for Pt obtained by other workers using the *ab initio* augmented plane wave (APW) method. The reason why the values of $(1 + \lambda_\gamma)$ obtained by other workers are so near to each other is due to the fact that they have all used a variation of the APW method. Our values are lower probably because we have absorbed a larger part of the many-body interactions by forcing a fit to the FS than the *ab initio* APW calculations. This again illustrates the arbitrariness in the $(1 + \lambda_\gamma)$ values obtained when different band calculations are used. We would like to stress that the same arbitrariness would also be present in the *ab initio* calculations of the electron-electron, electron-phonon and spin fluctuation interactions since they would also have to use a band structure. It would therefore be more meaningful to compare the three different values of the enhancement factor using the same band structure rather than to compare the same enhancement factor using different band structures.

5. λ_c using cyclotron data

We have calculated m_b for different orbits in Pd and Pt. These are calculated using our model. Values of the measured m_c for different orbits are given in tables 2 (for Pd) and

Table 1. Many-body mass enhancement factor, $1+\lambda_\gamma$ for Pd and Pt calculated from low temperature specific heat data. γ is in mJ/mole/K^2 and DOS is in state s/eV-atom-spin ($0{\cdot}2145\gamma$ = DOS at E_F).

Metal	References	Theoretical method	Expt.	Calc.	DOS expt.	DOS Calc.	$1+\lambda_\gamma$
Pd	a	RAPW	9·42	5·67			1·66
	b	RAPW	9·42		2·02	1·18	1·71
	c	RAPW	9·42		2·02	1·18	1·71
	d	Sp. Heat	9·2	5·5			1·7
	e	LAPW	9·42		2·02	1·28	1·58
	f	RAPW	9·42		2·02	1·14	1·77
	g	Interpolation	9·42		2·02	1·48	1·36
Pt	a	RAPW	6·56	4·02			1·63
	d	Sp. Heat	6·7	4·1			1·6
	e	LAPW	6·54		1·403	0·92	1·53
	g	Interpolation	6·54		1·403	1·15	1·22

a, Anderson (1970); b, Anderson and Mackintosh (1968); c, Christersen (1986); d, Knapp and Jones (1972); e, MacDonald *et al* (1981); f, Mueller *et al* (1970); g, present calculation.

Table 2. Mass enhancement factor $1+\lambda_c$ for Pd.

Field direction	Expt. m_c Dye *et al* 1981	$1+\lambda_c = m_c/m_b$
Γ-centred electrons		
⟨100⟩	2·02	1·28
⟨110⟩	2·30	1·45
⟨111⟩	1·96	1·26
X-centred holes		
⟨100⟩ XWU	−0·63	1·41
⟨110⟩ XUΓ	−1·03	1·25
⟨110⟩	−0·78	1·38
⟨111⟩	−0·87	1·42
L-centred hole		
⟨110⟩ LKΓ	−1·21	1·41
Open hole surface		
⟨100⟩ ε	10·96	1·36
⟨110⟩ β	−12·77	1·14
⟨110⟩ β	−5·7	1·09
⟨100⟩ α	−2·4	1·49

table 3 (for Pt). Using m_c and m_b we obtain λ_c. These are also given in tables 2 and 3. We notice that in one case $(1+\lambda_c)<1$. This is unphysical and casts doubts on the authenticity of the calculations. Our earlier work shows that these orbits are the same for which the fit of the FS was rather poor (in terms of% error). This leads to incorrect values of **k** and hence m_b. If we adjust E_F to fit these orbits and then calculate m_b, we find

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