

Supplement for “Polarization-dependent excitons and plasmon activity in nodal-line semimetal ZrSiS”

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Anisotropic effective masses

Let us consider a solid with a gap whose constant energy surfaces $\varepsilon(\mathbf{k})$ are ellipsoids, with effective masses $m_{\parallel}$ and $m_{\perp}$ for electrons and holes along the ellipsoid axis and in the plane perpendicular to it, respectively. In such a system, the binding energy of an exciton is given by

$$E(\lambda) = -\frac{3}{2} \left(\frac{e^2}{4\pi\varepsilon\hbar} \right)^2 \left(\frac{2}{\mu_{\perp}} + \frac{1}{\lambda^2\mu_{\parallel}} \right)^{-1} I(\lambda)^2, \quad (\text{S1})$$

where e is the electron charge, ε is the dielectric constant of the solid, $\hbar$ is the reduced Planck’s constant and $\mu_{\parallel}$ and $\mu_{\perp}$ are the reduced masses parallel and perpendicular to the ellipsoid axis, respectively. The function $I(\lambda)$ is given by

$$I(\lambda) = \frac{1}{2} \int_0^{\pi} \frac{\sin \theta d\theta}{\sqrt{1 + (\lambda^2 - 1) \cos^2 \theta}} = \begin{cases} \frac{\operatorname{arcsinh} \sqrt{\lambda^2 - 1}}{\sqrt{\lambda^2 - 1}} & \text{for } \lambda > 1 \\ \frac{\arcsin \sqrt{1 - \lambda^2}}{\sqrt{1 - \lambda^2}} & \text{for } \lambda < 1 \end{cases} \quad (\text{S2})$$

and λ is the solution of

$$\frac{\mu_{\perp}}{\mu_{\parallel}} = 2\lambda^2 \frac{1 - \lambda I(\lambda)}{I(\lambda) - \lambda} \quad (\text{S3})$$

Full details about this formalism can be found in [1]. In our case, the effective masses for the first excitons are summarized in Table S1 below.

According to this table, the binding energies for $\mathbf{E} \parallel Ox$ and $\mathbf{E} \parallel Oz$ are $E_b = 0.02E_0$ and $E_b = 0.16E_0$, where $E_b = -\frac{3}{2} \left(\frac{e^2}{4\pi\varepsilon\hbar} \right)^2$. These values indeed differ by a factor 8, as the main text indicates.

[1] A. Schindlmayr. Excitons with anisotropic effective mass. *Eur. J. Phys.*, 18:374–376, 1997.

$\boldsymbol{E} \parallel O x$							
	$m_{\perp,1}$	$m_{\perp,2}$	$m_{\perp} = \sqrt{m_{\perp,1} m_{\perp,2}}$	$m_{\parallel}$	$\mu_{\perp}$	$\mu_{\parallel}$	λ
Electrons	0.363	0.218	0.281	0.011	0.223	0.010	3.1417
Holes	4.611	0.257	1.089	0.136			
$\boldsymbol{E} \parallel O z$							
	$m_{\perp,1}$	$m_{\perp,2}$	$m_{\perp} = \sqrt{m_{\perp,1} m_{\perp,2}}$	$m_{\parallel}$	$\mu_{\perp}$	$\mu_{\parallel}$	λ
Electrons	0.609	3.718	1.505	1.134	0.576	0.378	1.162
Holes	0.261	3.342	0.933	0.567			

Table S1. Estimation of the λ parameter appearing in Eq. (S1).