Comment on “Electronic fine structure in the electron-hole plasma of SrB$_6$”

In a recent Letter \cite{1}, Rodriguez et al. addressed the origin of the high-temperature weak ferromagnetism found in doped hexaborides \cite{2} by calculating details of the band structure of SrB$_6$ in the vicinity of the X-point in the Brillouin zone. They conclude that crystal field induced electron-hole mixing has an important effect on the density of states (DOS) and suggest nesting between electron Fermi pockets as an alternative explanation to the excitonic ferromagnetism \cite{3}. We would like to question several conclusions in this work \cite{1}.

(i) Rodriguez et al. claim that the two bands cross only along the symmetry lines ($\xi, 0, 0$) and ($\frac{\pi}{3}, 0, 0$). This result contradicts a previous band structure study, which found band crossing in all symmetry planes passing through the X-point \cite{2}. The latter conclusion has a simple symmetry interpretation. At the X-point the valence and conduction bands belong to different irreducible representations of the small group: $X_3$, basis function $y_z$, and $X'_3$ symmetry, basis function $x(y^2-z^2)$, respectively. The band mixing occurs away from the X-point and is given by the product $X_3 \times X'_3$

$$\Delta_{\text{cryst}} \simeq E_b k_x k_y (k^2_y - k^2_z)/b^5,$$  \hspace{1cm} (1)

where $E_b$ is a bandwidth and $b = \frac{2\pi}{a}$ is a reciprocal lattice vector. The crystal field hybridization is strongly suppressed by the high power of momentum in Eq. (1) ($k_F \sim 0.1b$). Therefore, not only is the hybridization more anisotropic than suggested in Ref. \cite{1}, but also it is very weak on the scale of the band overlap. Our TB-LMTO calculations \cite{3} as well as FLAPW method \cite{5} yield an extremely small band mixing for a general direction in the Brillouin zone in agreement with Eq. (1).

(ii) Even for a strong hybridization, the DOS is quite different from the results of Ref. \cite{1}. Fig. 1 shows the DOS for two parabolic bands with anisotropic effective masses \cite{2,3}. band overlap $E_G = 100$ meV, and two angular dependences for the mixing matrix element: isotropic, which models an excitonic gap \cite{3}, and anisotropic given by Eq. (1). The amplitudes were chosen to give the same maximum splitting of $2\Delta_{\text{max}} = 15$ meV. Because of the anisotropic dispersion the DOS is slightly reduced at the Fermi level. The true gap in the DOS opens only for a sufficiently large excitonic gap $\Delta > 0.16E_G$. Note that the tetrahedron method for DOS does not allow for crossing of bands, which are numbered in increasing order of energy at every k-point, and, therefore, may lead to spurious peaks \cite{1} due to artificial anticrossings.

(iii) Correlation effects in the e-h plasma lead to a forbidden range for the band overlap values in the hexaborides \cite{2}. At the first order metal-insulator transition a semiconductor jumps into a dense plasma with $r_s \approx 1$. Rodriguez et al. have estimated $r_s = 2.5$ for the band overlap $E_G = 100$ meV in SrB$_6$, a value lying within the forbidden range. The real overlap must be larger. Therefore, the conclusion that 0.5% doping fills hole Fermi pockets in SrB$_6$ \cite{1}, which is based on the above underestimated value of $E_G$, is by no means reliable and does not exclude electron-hole pairing at this doping level.

(iv) Nesting of electron pockets between inequivalent X-points was suggested in Ref. \cite{1} as another source of CDW and SDW instabilities, which does not involve holes from the valence band. This suggestion is physically incorrect. The nesting condition refers to a sign change under translation in momentum space: $\epsilon(k+Q) \approx -\epsilon(k)$. Only in such a case can repulsive e-h interaction produce a density-wave instability in e-h channel, see e.g. \cite{7}.

Lastly, the interpretation of the de Haas-van Alphen measurements quoted in \cite{1} seems to us to be problematic in view of the high values of the low temperature resistivity reported for SrB$_6$ \cite{2} and its strong dependence on stoichiometry. Further information is required before a definitive conclusion can be made.

We thank R. Monnier for many useful discussions.

M. E. Zhitomirsky,$^1$ T. M. Rice,$^1$ and V. I. Anisimov$^2$

$^1$Theoretische Physik, ETH-Zürich, Switzerland
$^2$Institute of Metal Physics, Ekaterinburg, Russia

PACS numbers: 71.10.Hf, 71.18.+y, 75.10.Lp, 75.30.-m

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{dos.png}
\caption{The density of states in SrB$_6$ for two types of interband hybridization (a) isotropic excitonic gap, bold line, and (b) anisotropic crystal-field mixing Eq. (1), thin line.}
\end{figure}

[1] C. O. Rodriguez, R. Weht, and W. E. Pickett, Phys. Rev. Lett. 84, 3903 (2000).
[2] D. P. Young et al., Nature 397, 412 (1999).
[3] M. E. Zhitomirsky, T. M. Rice, and V. I. Anisimov, Nature 402, 251 (1999); cond-mat/9904333
[4] A. Hasegawa and A. Yanase, J. Phys. C 12, 5431 (1979).
[5] S. Massidda et al., unpublished (2000).
[6] M. E. Zhitomirsky and T. M. Rice, Phys. Rev. B 62, No. 3 (2000); cond-mat/9910272
[7] P. Fazekas, Lecture Notes on Electron Correlation and Magnetism, World Scientific (1999).
[8] H. R. Ott et al., Z. Phys. B 102, 83 (1997).