Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

An Accurate Computation of the de Haas-van Alphen frequencies and effective masses of $NbSe_2$ CHRISTOPHER HOWELLS, MICHELLE JOHANNES, IGOR MAZIN, Naval Research Laboratory — $NbSe_2$ is a layered superconducting material with a co-existing nearly commensurate CDW. Since both the CDW and superconducting transitions are related to a Fermi Surface instability, an accurate calculation of the Fermi Surface is essential for a microscopic understanding of the physical behavior of this compound. Here we demonstrate a novel computational method for calculating the dHvA frequencies and electron effective masses of $NbSe_2$. Our computational approach employs a FLAPW calculation of the $NbSe_2$ Fermi Surfaces using 40000 k-points. We extract the extremal cross sections (located in the Gamma-K-M and A-L-H planes) into a bitmap and then compute the dHvA frequencies from the number of pixels in the cross sections averaged over an extended Brilluoin zone. The effective masses are calculated by repeating this method with the Fermi energy shifted by 0.002 Ry. Our method satisfies Luttinger's theorem to within 0.1% - a full order of magnitude more accurate than previously published calculations. We use this accuracy to predict the dHvA frequencies and effective masses of $NbSe_2$ under pressure.

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Date submitted: 14 Dec 2005 Electronic form version 1.4