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Non-empirical Calculations of the upper-critical field H_{c2} for Nb, $NbSe_2$, and MgB_2 TAKAFUMI KITA, Division of Physics, Hokkaido University, MASAO ARAI, National Institute for Materials Science, Japan — Detailed Fermi-surface structures are essential to describe the upper critical field H_{c2} in type-II superconductors, as first noticed by Hohenberg and Werthamer [Phys. Rev. **153**, 493 (1967)] and shown explicitly by Butler for high- purity cubic Niobium [Phys. Rev. Lett. **44**, 1516 (1980)]. However, most of H_{c2} calculations performed so far have used simplified model Fermi surfaces and/or phenomenological fitting parameters. Due to this lack of *ab-initio*-type calculations, our understanding on H_{c2} remains at a rather unsatisfactory level. With these observations, we have derived an H_{c2} equation for classic type-II superconductors which is applicable to systems with anisotropic Fermi surfaces and/or energy gaps under arbitrary field directions. Based on the formalism, we have calculated H_{c2} curves for clean type-II superconductors Nb, $NbSe_2$, and MgB_2 using Fermi surfaces from *ab initio* electronic structure calculations. The results for Nb and $NbSe_2$ excellently reproduce both temperature and directional dependences of measured H_{c2} curves, including marked upward curvature of $NbSe_2$ near T_c. As for MgB_2, a good fit is obtained for a π/σ gap ratio of $\sim$0.3. Our results indicate essential importance of Fermi surface anisotropy for describing H_{c2}.

Takafumi Kita
Division of Physics, Hokkaido University

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