First-Principles Calculation of Coherence Length and Penetration Depth based on Density Functional Theory for Superconductors

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Keywords: density functional theory for superconductors, coherence length, penetration depth

The coherence length (ξ_0) and the magnetic penetration depth (λ_{L}) are the two fundamental length scales of a superconductor. They fix the upper critical field, the depairing current, and the classification into type I and type II, and are therefore central to assessing a material for applications. First-principles theory, however, has focused almost exclusively on the transition temperature (T_c). Density functional theory for superconducting (SCDFT) and Migdal-Eliashberg theory describe a spatially uniform, current-free superconducting state, from which neither length can be extracted. In practice ξ_0 and λ_{L} are obtained from Ginzburg-Landau (GL) theory, a macroscopic phenomenological framework whose material-dependent parameters must be supplied from experiment. A microscopic route to ξ_0 and λ_{L} on the same footing was demonstrated within dynamical mean-field theory [1], but a parameter-free scheme for real materials has been missing.

We therefore introduce into SCDFT [2] a singlet order parameter $\chi(\mathbf{r},\mathbf{r}') \equiv \langle \hat{\psi}_\uparrow(\mathbf{r})\,\hat{\psi}_\downarrow(\mathbf{r}')\rangle$ with finite center-of-mass momentum $\mathbf{Q}$,

$$\chi(\mathbf{r}+\mathbf{R},\mathbf{r}'+\mathbf{R}) = e^{i\mathbf{Q}\cdot\mathbf{R}}\,\chi(\mathbf{r},\mathbf{r}'),$$

which generalized Bloch theorem lets us treat in one unit cell. Solving the finite-$\mathbf{Q}$ gap equation gives the gap function $\Delta_{n\mathbf{k}}^{(\mathbf{Q})}$ for each Bloch orbital $(n,\mathbf{k})$ and the supercurrent; the calculation remains stable below 0.1% of the Brillouin zone. Near T_c the gap reproduces the asymptotic form obtained analytically in GL theory

$$\left\langle \Delta_{n\mathbf{k}}^{(\mathbf{Q})} \right\rangle_{\mathrm{FS}} = \left\langle \Delta_{n\mathbf{k}}^{(\mathbf{Q}=\mathbf{0})} \right\rangle_{\mathrm{FS}} \sqrt{1 - \xi_0^2\,|\mathbf{Q}|^2},$$

where $\langle\cdots\rangle_{\mathrm{FS}}$ denotes an average over the Fermi surface. The wave number at which it is suppressed determines ξ_0, and the supercurrent likewise gives λ_{L}; ξ_0, λ_{L}, and T_c thus follow from one theory without empirical input. For Al, In, Sn, Ta, Pb, Nb, V_3Si, and H_3S the results agree with experiment, including the type-I/type-II classification, and we construct the Uemura plot from first principles.

[1] N. Witt, *et al*., npj Quantum Mater. **9**, 100 (2024).
[2] M. Kawamura, T. Nomoto, N. Witt, and R. Arita, Phys. Rev. Lett. Accepted; arXiv:2603.05123.