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Theory of relativistic effects in superconductors

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Abstract

We develop a relativistic generalization of the Bogoliubov–de Gennes equations where the particle and hole amplitudes are Dirac spinors. In the weakly relativistic limit, we find, besides the usual spin–orbit, Darwin and kinetic energy corrections, additional 'spin–orbit' and 'Darwin' terms. These new terms are present in superconductors only and involve the pairing field in place of the electrostatic potential. They become relevant for superconductors such as the heavy-fermions and high-T_c compounds, which are characterized by a short coherence length and heavy elements in the lattice. © 1999 Elsevier Science B.V. All rights reserved.

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1. Introduction

Relativistic effects, such as spin–orbit coupling, are known to affect, e.g., the symmetry of the superconducting order parameter [1–3], the Knight shift [4], the value of the upper critical field [5,6], the magnetooptical response of superconductors [7,8] and the Cooper pair mass [9,10]. Previous work in the field mostly proceeded by ad hoc substitution of relativistic terms in the BCS equations, whenever deemed necessary. Clearly, such procedures are not failproof, and likely to miss terms arising from the subtle interplay of relativity and superconductivity. Recently, a systematic BCS-like theory of superconductivity, based on the Dirac equation, instead of the Schroedinger equation, was constructed [11,12]. One of the main results of that work, the so-called Dirac–Bogoliubov–de Gennes (DBdG) equation, is a relativistic generalization of the Bogoliubov–de Gennes equation. It reads

$$\begin{pmatrix} \hat{h}_\mathrm{d} & \hat{D} \\ -\hat{D}^* & -\hat{h}_\mathrm{d}^* \end{pmatrix} \begin{pmatrix} u_{jk} \\ v_{jk} \end{pmatrix} = E_{jk} \begin{pmatrix} u_{jk} \\ v_{jk} \end{pmatrix}. \qquad (1)$$

Here, $\hat{h}_\mathrm{d}$ is the Dirac Hamiltonian

$$\hat{h}_\mathrm{d} = \hat{\gamma}^0 \left[c\hat{\gamma} \cdot \boldsymbol{p} + mc^2 (1 - \hat{\gamma}^0) + q\hat{\gamma}^\mu A_\mu \right], \qquad (2)$$

where $\hat{\gamma}$ denotes the usual 4×4 Dirac matrices, and

$$\hat{D} = \int \mathrm{d}^3 r' \, \Delta(\boldsymbol{r}, \boldsymbol{r}') \ldots \hat{\eta} = \hat{d}\hat{\eta}. \qquad (3)$$

For a BCS superconductor, the matrix $\hat{\eta}$ is given by

$$\hat{\eta} = \begin{pmatrix} i\hat{\sigma}_y & 0 \\ 0 & i\hat{\sigma}_y \end{pmatrix}, \qquad (4)$$

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where $\hat{\sigma}_y$ is the second Pauli matrix. The nonrelativistic limit of Eq. (1) is the well-known Bogoliubov–de Gennes equation, while the nonsuperconducting limit reproduces the conventional Dirac equation for particles and holes. The weakly relativistic limit, obtained by expansion to second order in $1/c$, yields relativistic corrections to the conventional theory of superconductivity. Explicitly one finds

$$\left[\begin{pmatrix} \hat{h} & i\hat{\sigma}_y \hat{d} \\ -i\hat{\sigma}_y \hat{d}^* & -\hat{h}^* \end{pmatrix} + \frac{1}{4m^2c^2}\begin{pmatrix} \hat{h}_2 & \hat{d}_2 \\ \hat{d}_2^\dagger & -\hat{h}_2^* \end{pmatrix}\right] \times \begin{pmatrix} u_{jk} \\ v_{jk} \end{pmatrix} = E_{jk}\begin{pmatrix} u_{jk} \\ v_{jk} \end{pmatrix}. \quad (5)$$

Here, the first term is the standard Bogoliubov–de Gennes Hamiltonian in the presence of magnetic fields, with

$$\hat{h} = \frac{1}{2m}\left(\boldsymbol{p} - \frac{q}{c}\boldsymbol{A}(\boldsymbol{r})\right)^2 + V(\boldsymbol{r}) - \mu_0 \hat{\boldsymbol{\sigma}} \boldsymbol{B}(\boldsymbol{r}). \quad (6)$$

The term

$$\hat{h}_2 = \hbar \hat{\boldsymbol{\sigma}} (\nabla V(\boldsymbol{r})) \times \boldsymbol{p} + \frac{\hbar^2}{2} \nabla^2 V(\boldsymbol{r}) - \frac{\boldsymbol{p}^4}{2m}. \quad (7)$$

contains the conventional spin–orbit, Darwin and mass–velocity corrections of second order in $1/c$. The relativistic correction term $\hat{d}_2$ is written most conveniently in center-of-mass and relative coordinates, $\boldsymbol{s}(\boldsymbol{r},\boldsymbol{r}') = \boldsymbol{r} - \boldsymbol{r}'$ and $\boldsymbol{R}(\boldsymbol{r},\boldsymbol{r}') = (\boldsymbol{r} + \boldsymbol{r}')/2$. It then reads

$$\hat{d}_2 = \int \mathrm{d}^3 r' \Big[\hbar \hat{\boldsymbol{\sigma}} \cdot [\nabla_{\boldsymbol{R}} \Delta(\boldsymbol{s},\boldsymbol{R})] \boldsymbol{p}' + \frac{\hbar}{2} \hat{\boldsymbol{\sigma}} \cdot [\nabla_{\boldsymbol{s}} \Delta(\boldsymbol{s},\boldsymbol{R})] \boldsymbol{p}' + \frac{\hbar^2}{2} [\nabla_{\mathrm{R}}^2 \Delta(\boldsymbol{s},\boldsymbol{R})] \Big] \ldots i\hat{\sigma}_y. \quad (8)$$

The first two terms under the integral can be interpreted as counterparts to the conventional spin–orbit term, containing the pair-potential in place of the lattice potential, and gradients with respect to the center-of-mass and relative coordinates. Similarly, the last term can be regarded as a superconducting counterpart to the conventional Darwin term. These terms, which arise from the interplay between relativistic covariance and superconducting coherence, have been missed in all previous treatments of the subject.

2. Discussion

Several applications of this theory have been worked out: (i) The energy spectrum was calculated for homogeneous superconductors. A small shift of the position of the gap with respect to the nonrelativistic value was predicted [11]. (ii) A complete symmetry classification of all possible order parameters consistent with the requirement of relativistic covariance has been worked out [12]. The classification was performed both with respect to the transformation behaviour under Lorentz transformations and with respect to the discrete symmetries of the underlying pair states. It turns out that the relativistic theory allows more different order parameters than the nonrelativistic theory. (iii) The spin–orbit terms were used as basic ingredients in our recent analysis of magnetooptical effects in superconductors. The absorption of polarized light by superconductors was found to be strongly modified by relativistic effects [7,8]. The predictions made for the magnetooptical response are consistent with recent experiments. Our theory is also consistent with the experimentally observed relativistic mass correction to the Cooper pair [9,10]. Further applications are currently being worked out in the fields of dichroism in vortices and relativistic effects in SNS multilayers. In these systems, the pair-potential has large spatial variations, so we expect the relativistic correction terms involving the gradients of the pair-potential to give important contributions.

3. Conclusion

If all relativistically allowed order parameters are to be included in Eq. (1), one needs 15 further matrices, in addition to $\hat{\eta}$. These matrices correspond to the relativistic generalizations of the triplet order parameters as well as to new types of order parameters, not known from the nonrelativistic case [12]. A weakly relativistic approximation then yields relativistic corrections to triplet superconductivity and, additionally, a new class of relativistic corrections, which are of first order in $1/c$ [13]. These terms are currently under study.

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