
Density Functional Theory for Superconductors

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ABSTRACT: Two recently proposed exchange-correlation functionals describing the superconducting phase of matter are reviewed and further explored: Whereas the first is a generalization of the local density approximation dealing with purely electronic correlations, the second is a functional derived from Kohn–Sham perturbation theory that includes electronic and phononic correlations on the same footing. Superconducting properties of simple metals obtained with the latter functional agree rather well with experimental results. © 2004 Wiley Periodicals, Inc. *Int J Quantum Chem* 99: 790–797, 2004

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Introduction

One of the most successful theories introduced in condensed matter physics and theoretical chemistry is density functional theory (DFT). Its foundations were established in the mid-1960s in

two seminal articles by Hohenberg and Kohn [1] and Kohn and Sham [2]. The first proved rigorously that all physical observables—such as the ground-state energy—can be written as functionals of the electronic density. This is a nontrivial statement and quite surprising at first sight. To completely describe the ground state of a many-body system one does not require knowledge of the complicated many-body wave function, but only that of a simple three-dimensional function: the density. In the sec-

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ond article, Kohn and Sham introduced a scheme to obtain the density from the solution of a fictitious noninteracting electronic system. These noninteracting electrons move in a local potential that includes, apart from the external field, the classical electrostatic interaction, and an exchange and correlation (xc) term that accounts for all the many-body effects. To approximate the latter quantity, they proposed the famous local density approximation (LDA). Despite its simplicity, the LDA performs remarkably well in a huge variety of molecular and solid-state systems. Over the next three decades, several other xc functionals were proposed in the literature. Today, with the most modern generalized gradient approximations (GGA) or orbital functionals, DFT can compete with the computationally much more intensive quantum-chemistry methods, and is the method of choice for large systems.

Unfortunately, not all physical properties can be easily written as functionals of the ground-state density—e.g., excitation energies or properties of the superconducting state. Several extensions of the basic theory have been put forward to remedy this inconvenience. In this article, we describe some recent advances of one of those extensions, namely, DFT for superconductors (SCDFT). The basic Hohenberg–Kohn and Kohn–Sham theorems of SCDFT were proved by Oliveira, Gross, and Kohn in the late 1980s [3]. However, very few applications of the theory have appeared in the literature [4], primarily because of the lack of reliable xc functionals.

The first attempt to construct such a functional was a generalization of the LDA to the superconducting case [5]. This functional only accounts for the purely electronic correlations in superconductors and is based on the xc energy of a uniform electron gas made superconducting by an external pairing field. To calculate the latter quantity, the authors proposed the use of Kohn–Sham perturbation theory at the level of a random-phase approximation (RPA) [6]. Recently, a new functional incorporating both the electron–electron and electron–phonon interactions was obtained [7] by using a method resembling the optimized effective potential method. The superconducting transition temperatures and the gaps at zero temperature, calculated for simple metals within this formalism, turn out to agree well with experiment.

In our opinion, SCDFT has now attained a level of maturity that allows it to compete with the traditional many-body approaches [8, 9, 10]. Its two main advantages are the relative simplicity of the

SCDFT equations, and the nonexistence of any semiphenomenological parameter such as the μ^* of Eliashberg theory [9].

This article is structured as follows: In the next section we provide a succinct description of SCDFT presenting the basic equations of the theory. We then describe the construction of xc functionals for superconductors. First, we present the LDA functional of Ref. [5]. To visualise this functional, the anomalous Hartree and the xc energies of the uniform superconducting electron gas are evaluated for a variety of order parameters. In the last section, we describe the calculation of material-specific properties of superconductors, using the functional of Ref. [7]. We conclude with a brief outlook.

DFT for Superconductors

We will begin with a brief overview of the SCDFT equations. This generalization of normal DFT to study superconductivity uses two densities: the normal electronic density

$$n(\mathbf{r}) = \sum_{\sigma} \langle \hat{\Psi}_{\sigma}^{\dagger}(\mathbf{r}) \hat{\Psi}_{\sigma}(\mathbf{r}) \rangle, \quad (1)$$

and the “anomalous” density

$$\chi(\mathbf{r}, \mathbf{r}') = \langle \hat{\Psi}_{\uparrow}(\mathbf{r}) \hat{\Psi}_{\downarrow}(\mathbf{r}') \rangle, \quad (2)$$

which is the order parameter characterizing the superconducting phase. In the previous expressions, the field operator $\hat{\Psi}_{\sigma}(\mathbf{r})$ annihilates an electron of spin σ ($\sigma = \uparrow, \downarrow$) at the position \mathbf{r} . With these densities, a Hohenberg–Kohn theorem is easily established [3] by generalizing Mermin’s arguments [11] for DFT at finite temperature. The theorem states that there is a one-to-one correspondence between the pair of external potentials $\{v - \mu, \Delta\}$ and the pair of equilibrium densities $\{n, \chi\}$. $\Delta(\mathbf{r}, \mathbf{r}')$ represents an external pairing field while $v(\mathbf{r})$, as in ordinary DFT, is a local potential, and μ is the chemical potential. The thermodynamic potential, as well as all other observables, can thus be written as a functional of $\{n, \chi\}$. The next step is the construction of a noninteracting Kohn–Sham Hamiltonian

$$\hat{H}_s = \sum_{\sigma} \int d^3r \hat{\Psi}_{\sigma}^{\dagger}(\mathbf{r}) \left[-\frac{\nabla^2}{2} + v_s(\mathbf{r}) - \mu_s \right] \hat{\Psi}_{\sigma}(\mathbf{r}) - \left[\int d^3r \int d^3r' \Delta_s^*(\mathbf{r}, \mathbf{r}') \hat{\Psi}_{\uparrow}(\mathbf{r}) \hat{\Psi}_{\downarrow}(\mathbf{r}') + \text{H.c.} \right]. \quad (3)$$

Atomic units are used throughout in all equations. The Kohn–Sham electrons are subject to an effective local potential, $v_s(\mathbf{r})$, and to an effective pair potential, $\Delta_s(\mathbf{r}, \mathbf{r}')$, chosen in such a way that the densities of the Kohn–Sham system equal the densities of the interacting system. Diagonalizing this Hamiltonian leads to the Bogoliubov–de Gennes-type equations

$$\begin{aligned} \left[-\frac{\nabla^2}{2} + v_s(\mathbf{r}) - \mu_s \right] u_i(\mathbf{r}) + \int d^3r' \Delta_s(\mathbf{r}, \mathbf{r}') v_i(\mathbf{r}') \\ = E_i u_i(\mathbf{r}) \\ - \left[-\frac{\nabla^2}{2} + v_s(\mathbf{r}) - \mu_s \right] v_i(\mathbf{r}) + \int d^3r' \Delta_s^*(\mathbf{r}, \mathbf{r}') u_i(\mathbf{r}') \\ = E_i v_i(\mathbf{r}), \quad (4) \end{aligned}$$

where u_i and v_i are the electron and hole amplitudes, and the Kohn–Sham potentials are defined as

$$v_s[n, \chi](\mathbf{r}) = v_0(\mathbf{r}) + v_H[n](\mathbf{r}) + v_{xc}[n, \chi](\mathbf{r}) \quad (5)$$

$$\begin{aligned} \Delta_s[n, \chi](\mathbf{r}, \mathbf{r}') = \Delta_0(\mathbf{r}, \mathbf{r}') + \Delta_H[\chi](\mathbf{r}, \mathbf{r}') \\ + \Delta_{xc}[n, \chi](\mathbf{r}, \mathbf{r}'). \quad (6) \end{aligned}$$

$v_0(\mathbf{r})$ represents the external Coulomb potential generated by the periodic lattice of the ions, while $\Delta_0(\mathbf{r}, \mathbf{r}')$ usually vanishes unless there is an external pairing field produced by the proximity of an adjacent superconductor. In these expressions, and in the following, the square brackets indicate a functional dependence. Note that the xc potentials v_{xc} and Δ_{xc} are functionals of both the normal and the anomalous density, whereas the Hartree potentials, v_H and Δ_H , depend only on one density and are defined as

$$v_H[n](\mathbf{r}) = \int d^3r' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}, \quad (7)$$

$$\Delta_H[\chi](\mathbf{r}, \mathbf{r}') = -\frac{\chi(\mathbf{r}, \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}. \quad (8)$$

The xc potentials are defined as functional derivatives of the xc free energy functional, F_{xc}

$$v_{xc}[n, \chi](\mathbf{r}) = \frac{\delta F_{xc}[n, \chi]}{\delta n(\mathbf{r})} \quad (9)$$

$$\Delta_{xc}[n, \chi](\mathbf{r}, \mathbf{r}') = -\frac{\delta F_{xc}[n, \chi]}{\delta \chi^*(\mathbf{r}, \mathbf{r}')}. \quad (10)$$

In principle, these potentials include all many-body effects induced by electron–electron and electron–phonon interactions. The functional dependence of F_{xc} on the densities can be extremely complicated and has to be approximated in any practical application of the theory.

To simplify the previous equations we introduce the so-called decoupling approximation [12] for u_i and v_i

$$u_i(\mathbf{r}) \approx u_i \varphi_i(\mathbf{r}), \quad v_i(\mathbf{r}) \approx v_i \varphi_i(\mathbf{r}), \quad (11)$$

where φ_i are solutions of the normal-state Kohn–Sham equation. The eigenvalues of Eq. (4) are then given by $E_i = \pm \sqrt{\xi_i^2 + |\Delta_i|^2}$, with $\xi_i = \epsilon_i - \mu_s$, and ϵ_i are the Kohn–Sham eigenvalues corresponding to φ_i . The solution of the normal-state Kohn–Sham equation can be achieved using standard band-structure methods. Finally, Δ_i is defined as

$$\Delta_i = \int d^3r \int d^3r' \varphi_i^*(\mathbf{r}) \Delta_s(\mathbf{r}, \mathbf{r}') \varphi_i(\mathbf{r}'). \quad (12)$$

The decoupling approximation reduces the problem to the solution of a BCS-like gap equation

$$\Delta_i = -Z_i[\Delta_s] \Delta_i - \frac{1}{2} \sum_j \frac{\tanh\left(\frac{\beta}{2} E_j\right)}{E_j} K_{ij}[\Delta_s] \Delta_j, \quad (13)$$

where β is the inverse temperature. The kernel of the gap equation is divided into two parts: a purely diagonal term, Z_i , and a nondiagonal part, K_{ij} , both being functionals of the Kohn–Sham pairing potential Δ_s . This equation has the same structure as the BCS gap equation, with the K_{ij} kernel playing the role of the model interaction kernel and Z_i playing a role similar to the renormalization term in the Eliashberg equations. This similarity allows us to interpret the quantity $K_{ij}/(1 + Z_i)$ as an effective

interaction responsible for the binding of the Cooper pairs.

Local Density Approximation for Superconductors

The LDA functional for superconductors (SCLDA) [5] can be constructed in an analogy to the local spin density approximation (LSDA), with the anomalous density playing the role of the spin-magnetization density in LSDA. Whereas the LSDA is derived from the xc energy of a uniform electron gas exposed to a constant magnetic field, the input required by the SCLDA is the xc energy of the uniform electron gas under the influence of a homogeneous external pairing potential. Because of the translational invariance of the gas, it is convenient to work in momentum space. The xc energy per unit volume of the uniform gas will then be a *function* of the normal density n and a *functional* of the anomalous density $\chi(\mathbf{k})$, i.e.,

$$f_{xc}^{\text{hom}} = f_{xc}^{\text{hom}}[n, \chi(\mathbf{k})]. \quad (14)$$

With the help of this quantity, we define the LDA for superconductors as

$$F_{xc}^{\text{SCLDA}}[n(\mathbf{R}), \chi(\mathbf{R}, \mathbf{k})] = \int d^3R f_{xc}^{\text{hom}}[n, \chi(\mathbf{k})]_{\chi(\mathbf{k}) = \chi_W(\mathbf{R}, \mathbf{k})}^{n=n(\mathbf{R})} \quad (15)$$

where $\chi_W(\mathbf{R}, \mathbf{k})$ is the Wigner transform of the anomalous density of the inhomogeneous system, given by

$$\chi_W(\mathbf{R}, \mathbf{k}) = \int d^3s e^{i\mathbf{k}\cdot\mathbf{s}} \chi\left(\mathbf{R} + \frac{\mathbf{s}}{2}, \mathbf{R} - \frac{\mathbf{s}}{2}\right), \quad (16)$$

where \mathbf{R} represents the center of mass of the Cooper pair, $\mathbf{R} = (\mathbf{r} + \mathbf{r}')/2$, and \mathbf{s} represents the relative coordinate, $\mathbf{s} = \mathbf{r} - \mathbf{r}'$. Although other forms for the SCLDA might be conceivable, we can show that Eq. (15) is the *only* correct definition. This is achieved by performing a semiclassical expansion of the total energy [13]. Then the lowest-order terms in \hbar are identical with the SCLDA.

The quantity f_{xc}^{hom} is essential in this functional. Various methods could be used to obtain it, e.g., quantum Monte Carlo, or many-body perturbation

theory. We will use the latter to write the xc energy of the electron gas as a series expansion in powers of e^2 , where e is the electron charge. In first order in e^2 , one finds

$$f_x = -\frac{1}{4} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \frac{4\pi}{|\mathbf{k} - \mathbf{k}'|^2} \times \left[1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \tanh\left(\frac{\beta}{2} E_{\mathbf{k}}\right)\right] \left[1 - \frac{\xi_{\mathbf{k}'}}{E_{\mathbf{k}'}} \tanh\left(\frac{\beta}{2} E_{\mathbf{k}'}\right)\right]. \quad (17)$$

This term is the generalization of the normal exchange energy. In second order, we find that some of the contributions diverge. This well-known behavior is caused by the long-range nature of the Coulomb interaction. To remedy this problem, one can resort to infinite resummations of the perturbation series, the simplest of which is the so-called random-phase approximation (RPA) [6]. In the context of this article, the RPA energy can be written as

$$f_c^{\text{RPA}} = \frac{1}{2\beta} \int \frac{d^3q}{(2\pi)^3} \sum_{\nu_n} \log[1 - v(q, \nu_n) \Pi_0(\mathbf{q}, \nu_n)] + v(q, \nu_n) \Pi_0(\mathbf{q}, \nu_n), \quad (18)$$

where the irreducible polarization propagator, Π_0 , is defined by

$$\Pi_0(\mathbf{q}, \nu_n) = \frac{2}{\beta} \int \frac{d^3k}{(2\pi)^3} \sum_{\omega_n} [G(\mathbf{k}, \omega_n) \times G(\mathbf{k} + \mathbf{q}, \omega_n + \nu_n) + F(\mathbf{k}, \omega_n) F^\dagger(\mathbf{k} + \mathbf{q}, \omega_n + \nu_n)]. \quad (19)$$

Here, ω_n and ν_n are odd and even Matsubara frequencies, respectively. G , F , and F^\dagger represent the normal and anomalous Green's functions of the superconducting electron gas [5].

In ordinary DFT the xc energy for the electron gas is a simple function of the density. One can therefore evaluate $f_{xc}^{\text{hom}}(n)$ for a set of densities, and fit the result to some analytic form. As already mentioned, f_{xc}^{hom} for the superconducting electron gas is a functional of $\chi(\mathbf{k})$, so even if we could calculate it, we could not fit the results in terms of simple parameters. To circumvent this problem, we parametrize the anomalous density (or equivalently the pair potential), thereby transforming the xc functional into a much simpler function of the expansion coefficients. As a first step, we investigate

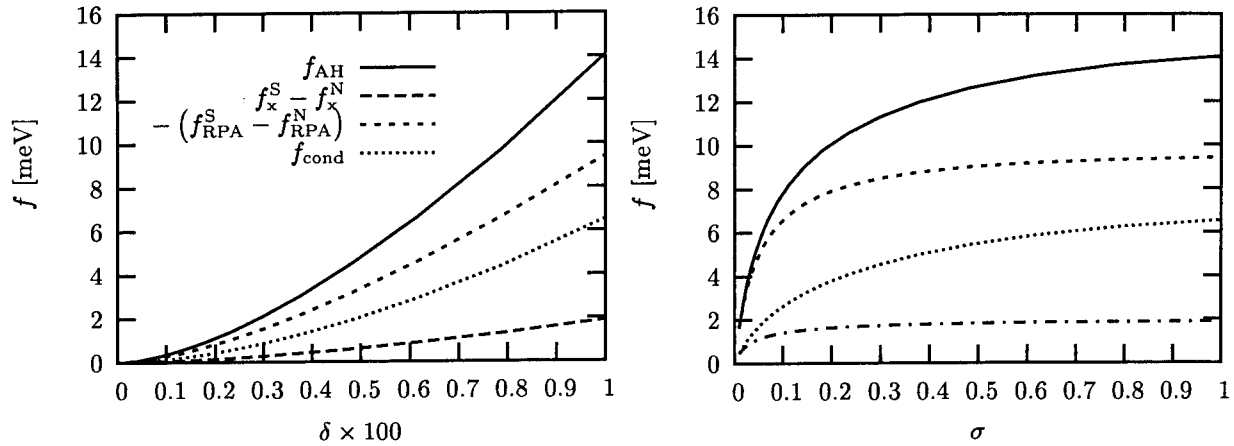


FIGURE 1. Energies vs δ for an s-wave pair-potential with $\sigma = 1$ (left panel) and energies vs σ for a pair-potential with $\delta = 0.01$ (right panel). Both panels were calculated for $r_s = 1$ and $T = 0$ K.

the functional for an s-wave pairing potential having the shape of a Gaussian

$$\Delta_s(\mathbf{k}) = \mu_s \delta \exp\left[\frac{(k/k_F - 1)^2}{\sigma^2}\right] \quad (20)$$

where k_F is the Fermi momentum, and δ and σ are dimensionless parameters. To gain some insight into the relative importance of the anomalous Hartree energy [the energy term associated with the anomalous Hartree potential (8)]

$$f_{\text{AH}} = \frac{1}{4} \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \frac{4\pi}{|\mathbf{k} - \mathbf{k}'|^2} \frac{\Delta(\mathbf{k})}{E_{\mathbf{k}}} \frac{\Delta(\mathbf{k}')}{E_{\mathbf{k}'}} \times \tanh\left(\frac{\beta}{2} E_{\mathbf{k}}\right) \tanh\left(\frac{\beta}{2} E_{\mathbf{k}'}\right), \quad (21)$$

versus the exchange and the RPA contributions, we calculated these quantities numerically for a wide range of parameters.

The results are summarized in Figure 1, where we plot the difference of exchange energies, $f_x^S - f_x^N$, in the superconducting (S) and normal (N) states; the negative difference $-(f_{\text{RPA}}^S - f_{\text{RPA}}^N)$ of the corresponding RPA correlation energies; the anomalous Hartree energy, f_{AH} and the sum, f_{cond} , of these three terms representing the potential part of the condensation energy. In the left panel of Figure 1 these energies are plotted versus the parameter δ for $\sigma = 1$, and in the right panel the same quantities are plotted as functions of σ for $\delta = 0.01$. These two plots were obtained for $r_s = 1$. The temperature in

this calculation was set to zero. The dependence of the energies on the parameters σ and δ turns out to be rather smooth. The largest positive contribution comes from the anomalous Hartree term, and is almost canceled by the RPA correlation energy difference ($f_{\text{RPA}}^S - f_{\text{RPA}}^N$). The exchange part is positive, but much smaller (almost an order of magnitude) than the other two terms. The sum of the three is positive everywhere. The same statement holds true for $0.01 \leq \delta \times 100 \leq 1$, $0.01 \leq \sigma \leq 1$, and $r_s = 0.1, 1, 2, 3, 4, 5$. In the conventional s-wave superconductors, the pairing mechanism is phononic, and the above Coulombic positive-energy contributions reduce superconductivity.

Phonon-Induced Superconductivity

For a proper description of real materials, both the electron–phonon and electron–electron interactions have to be included. A suitable xc functional has been constructed via Kohn–Sham perturbation theory taken to the second order in powers of e , the electron charge, and g , the electron–phonon coupling constant. The resulting gap equation was then simplified by taking the values of K_{ij} and Z_i at $\Delta = 0$. Two terms were found to contribute to the kernel K_{ij} , the first of phononic origin, K_{ij}^{ph} , and the second of electronic origin, K_{ij}^{el} . They can be written as

$$K_{ij}^{\text{el}} = w_{ij},$$

$$K_{ij}^{\text{ph}} = \frac{2}{\tanh\left(\frac{\beta}{2}\xi_i\right)\tanh\left(\frac{\beta}{2}\xi_j\right)} \sum_{\epsilon\mathbf{q}} |g_{\epsilon\mathbf{q}}^{ij}|^2 \times [I(\xi_i, \xi_j, \Omega_{\epsilon\mathbf{q}}) - I(\xi_i, -\xi_j, \Omega_{\epsilon\mathbf{q}})] \quad (22)$$

where w_{ij} is the matrix element of the Coulomb interaction

$$w_{ij} = \int d^3\mathbf{r} \int d^3\mathbf{r}' \varphi_i^*(\mathbf{r})\varphi_i(\mathbf{r}') \frac{1}{|\mathbf{r} - \mathbf{r}'|} \varphi_j^*(\mathbf{r})\varphi_j(\mathbf{r}'). \quad (23)$$

$g_{\epsilon\mathbf{q}}^{ij}$ is the electron–phonon coupling constant, $\Omega_{\epsilon\mathbf{q}}$ the phonon frequency, and ϵ and \mathbf{q} are the phonon

polarization and wave-vector, respectively. The function I is defined as

$$I(\xi_i, \xi_j, \Omega_{\epsilon\mathbf{q}}) = f_{\beta}(\xi_i) f_{\beta}(\beta_j) n_{\beta}(\Omega_{\epsilon\mathbf{q}}) \times \left(\frac{e^{\beta\xi_i} - e^{\beta(\xi_j + \Omega_{\epsilon\mathbf{q}})}}{\xi_i - \xi_j - \Omega_{\epsilon\mathbf{q}}} - \frac{e^{\beta\xi_i} - e^{\beta(\xi_j + \Omega_{\epsilon\mathbf{q}})}}{\xi_i - \xi_j + \Omega_{\epsilon\mathbf{q}}} \right), \quad (24)$$

where f_{β} and n_{β} are the Fermi–Dirac and the Bose–Einstein distribution functions, respectively.

Similarly, two terms contribute to Z_i ,

$$Z_i^{\text{el}} = -\frac{1}{2\xi_i} \left\{ \sum_j w_{ij} \left[1 - \tanh\left(\frac{\beta}{2}\xi_j\right) \right] - \frac{\sum_{jk} \frac{\beta}{2} w_{jk} \left[1 - \tanh\left(\frac{\beta}{2}\xi_k\right) \right]}{\sum_j \frac{\beta}{2} \frac{1}{\cosh^2\left(\frac{\beta}{2}\xi_j\right)}} \right\} \quad (25)$$

$$Z_i^{\text{ph}} = \frac{2}{\tanh\left(\frac{\beta}{2}\xi_i\right)} \sum_j \sum_{\epsilon\mathbf{q}} |g_{\epsilon\mathbf{q}}^{ij}|^2 I'(\xi_i, \xi_j, \Omega_{\epsilon\mathbf{q}}), \quad (26)$$

where I' is the derivative of I with respect to its first argument.

It is a demanding numerical task to obtain the gap as a function of \mathbf{k} , for it involves the solution of a three-dimensional integral equation. This is required if one wants to study the angular anisotropy of the gap, or if the Fermi surface of the material is highly nonspherical. However, for the simple systems we consider in this work, the calculations can be simplified by approximating the electronic eigenspectrum with a free-electron parabola, and by assuming the electron–phonon coupling constant to be independent of \mathbf{k} . These approximations allow us to convert the three-dimensional gap equation into a one-dimensional integral equation by changing the variable of integration from wave-vector to energy. In addition, to take into account screening effects, we replaced the bare Coulomb interaction by a Thomas–Fermi function.

To solve numerically the nonlinear gap equation (13) for different temperatures, we iterate it until convergence is achieved. No more than a few hun-

dred iterations were necessary, which corresponds to a few minutes of computer time for every given temperature. In Figure 2, we show typical solutions of the gap equation at 0.01 K for two different metals, tantalum and aluminum. In the same figure we show the dependence of the gap at the Fermi energy, Δ_0 , on the temperature.

To find the precise value of the critical temperature, T_c , we followed a simpler and numerically more stable procedure: The gap equation was linearized in Δ and converted into an eigenvalue problem by introducing the “eigenvalue” λ

$$\lambda(\beta)\Delta_i = \sum_j M_{ij}\Delta_j, \quad (27)$$

where i denotes the mesh index, and M is defined as

$$M_{ij} = -\frac{1}{2} \frac{K_{ij}[\Delta = 0]}{1 + Z_i[\Delta = 0]} \frac{\tanh\left(\frac{\beta\xi_i}{2}\right)}{\xi_i}. \quad (28)$$

In this way, T_c is identified as the temperature for which the largest eigenvalue $\lambda^{\text{max}}(\beta)$ is equal to

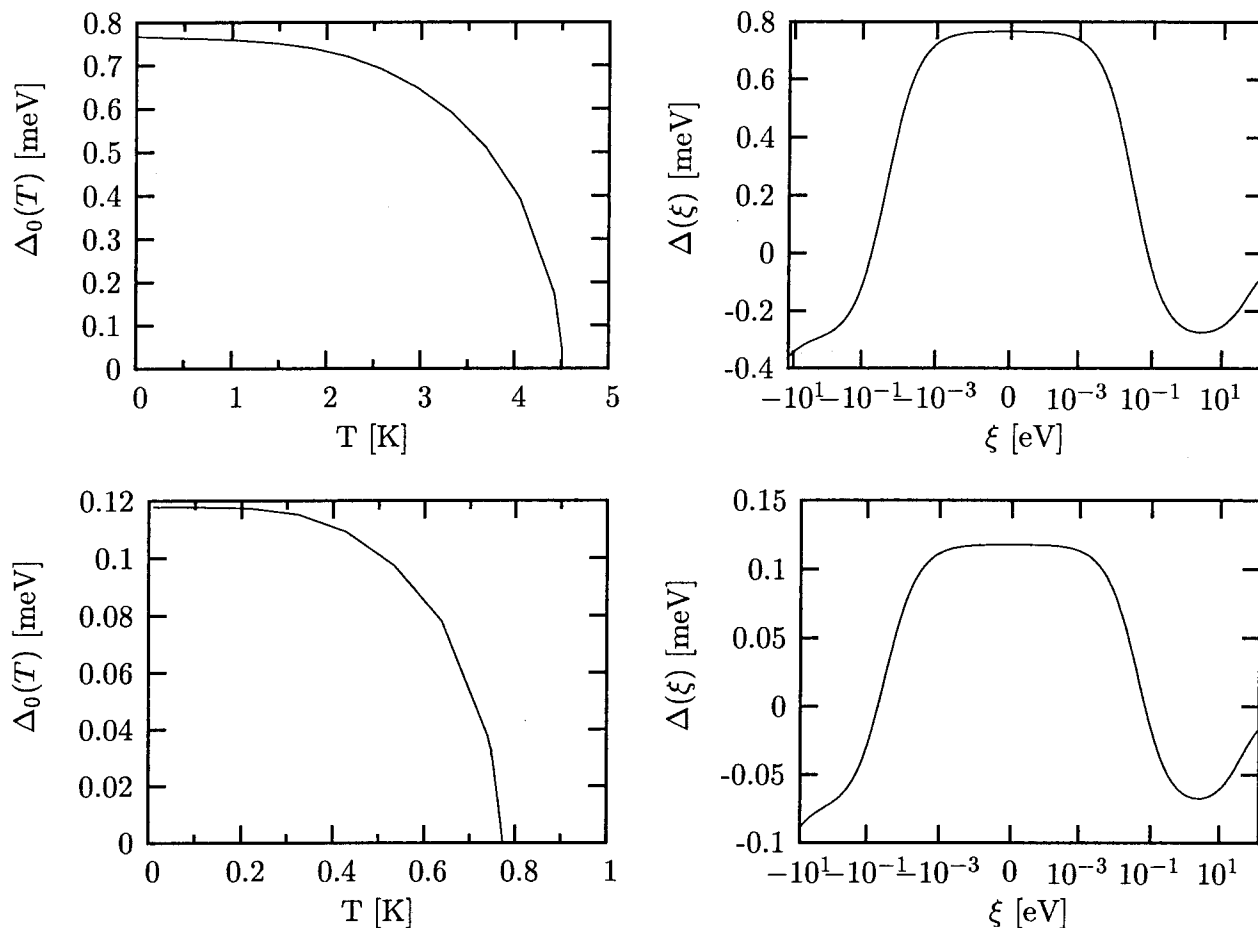


FIGURE 2. Temperature dependence of the gap function at the Fermi energy, Δ_0 , and the gap vs energy at zero temperature for tantalum (upper panels) and aluminum (lower panels).

one. As we are only interested in the dominant eigenvalue of M , we simply iterate Eq. (27) until self-consistency is reached. It is then simple to prove that

$$\lambda^{\max}(\beta) = \frac{\sum_j M_{ij}^{\infty} \Delta_j^{\infty}}{\Delta_i^{\infty}}. \quad (29)$$

The equation $\lambda(\beta) = 1$ is then solved by a simple bisection algorithm.

Our findings for T_c and Δ_0 are shown in Table I. The electron-phonon coupling constants, $g_{\epsilon q}$, used to obtain these results were calculated from first principles in Ref. [15]. Given that both T_c and Δ_0 depend extremely sensitively on the electron-phonon coupling constants, the agreement between the calculated values and the experiment is remarkably good. Both T_c and Δ_0 are overestimated for vanadium, an expected result due to the strong spin

fluctuations existing in this material, which our present functional does not take into account. The small values of T_c and Δ_0 for aluminum and mo-

TABLE I
Computed transition temperatures (in K) and superconducting gaps at zero temperature (in meV) for simple metals compared with experimental values from Ref. [14].

	T_c (DFT)	T_c (exp.)	Δ_0 (DFT)	Δ_0 (exp)
Al	0.76	1.18	0.117	0.179
Nb	9.37	9.5	1.69	1.55
Mo	0.65	0.92	0.099	—
Ta	4.51	4.48	0.764	0.694
V	16.3	5.38	2.99	0.789
Pb	6.58	7.2	1.24	1.33
Cu	<0.01	—	—	—

lybdenum, on the other hand, indicate a systematic underestimation of the phononic part of the kernel, K_{ij}^{ph} , for small temperatures. We emphasize that there are no phenomenological parameters involved in the calculation. All quantities are calculated from first principles. The results represent the first fully ab initio calculations of material-specific properties of superconductors. The rather good agreement with experiment is certainly encouraging. The next step toward the description of more complex superconductors, with band structures deviating strongly from spherical symmetry, will be the implementation of the three-dimensional gap equation.

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