Effect of spin fluctuations on $T_c$ from density-functional theory for superconductors.

Małgorzata Wierzbowska
INFM DEMOCRITOS National Simulation Center, via Beirut 2–4, 34014 Trieste, Italy

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Abstract. The transverse spin fluctuations are introduced to the density functional theory for superconductors (SCDFT). Paramagnons are treated within the random phase approximation and assumed to be the same for the normal and superconducting state. The effect of spin fluctuations on $T_c$ is studied for a few simple metals at ambient pressure and niobium at several pressures up to 80 GPa.

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1 Introduction

Since the discovery of superconductivity many theories have been born to explain this phenomenon and calculate observables. First papers about the role of spin fluctuations by Doniach and Engelsberg [1] and Izuyama et al. [2] were published in sixties. Till today, fluctuations have been introduced to many-body and phenomenological models and a very popular semiempirical theory proposed by Eliashberg [3].

The goal of this work is to include the spin fluctuations into the density functional theory for superconductors which, in principle, enables to calculate all material properties, also in the superconducting state, from first principles. The framework of the SCDFT was set up by Oliveira, Gross and Kohn [4] in 1988. Recently, the SCDFT gap equation has been solved numerically for simple metals [5,6] and MgB$_2$ [7].

As for the critical temperatures, it is known for a long time, that spin fluctuations decrease considerably $T_c$ of some superconductors [8,9]. In our previous work for niobium under pressure [10], we solved the gap equation of the Eliashberg theory [3] with and without spin fluctuations and the SCDFT gap equation only with the Coulomb and phonon interactions. We found that the effect of paramagnons decreased $T_c$ obtained from the Eliashberg theory by 3-4 K, however, an approximate treatment of the Coulomb interactions by a simple constant, $\mu^*$, led to a large disagreement of the theoretical results with the experimental data [11]. In contrast to the Eliashberg theory, the SCDFT scheme is parameter free, but the critical temperature calculated without spin fluctuations for Nb at ambient pressure [10] was about 3.7 K higher than the experimental $T_c$.

In this work, we follow the derivations of the SCDFT gap equation given in a number of PhD theses [12,13,14] and we include the spin fluctuations. The paramagnon spectral function is calculated within the random phase approximation (RPA) with the assumption of the homogeneous electron gas, similarly to the work by Berk and Schrieffer [8] done for the Eliashberg theory. We solve the obtained gap equation for a few simple metals and update our previous results for niobium under pressure.

In the following Sections, we introduce the SCDFT gap equation and the construction of the exchange-correlation functional, $F_{xc}$, by collecting the most important building blocks of the theory given by its authors [4] and first developers [12,13,14,15]. These sections are: II. SCDFT gap equation, III. Exchange-correlation functional, and IV. Coulomb interaction and phonons in $F_{xc}$. Above Sections are written using the notation according to Parks [17], [18] and Vonsovsky [19]. This notation is in some points, such as Nambu Green’s function and the selfenergy, different than the notation previously used for the SCDFT [12,13,14]. We introduce the spin fluctuations in Sections: V. Paramagnons in $F_{xc}$ and VI. Gap equation with paramagnons and implementation details. We report obtained critical temperatures in Section VII, and we summarize in Section VIII.

2 SCDFT gap equation

In this Section, we wish to guide the reader, step by step, to the gap equation which will be solved at the end of this work to calculate the critical temperatures. We start by bringing the fundamentals of the SCDFT [4] and the
The grand-canonical Hamiltonian for a superconductor reads

\[ \hat{H}_{v,\Delta} = \sum_{\sigma} \int d^3r \left[ \frac{-\nabla^2}{2} + v(r) - \mu \right] \hat{\psi}_{\sigma}(r) + \frac{1}{2} \int d^3r d^3r' \hat{\psi}_{\sigma}^\dagger(r) \frac{1}{|r-r'|} \hat{\psi}_{\sigma}(r') \hat{\psi}_{\sigma}(r) \]

\[ - \int d^3r_1 d^3r'_1 d^3r_2 d^3r'_2 \hat{\psi}_{\sigma}^\dagger(r'_1) \hat{\psi}_{\sigma}(r_2) \times w(r'_1, r_1, r_2, r'_2) \hat{\psi}_{\sigma}(r_2) \hat{\psi}_{\sigma}(r_1) \]

\[ - \left[ \int d^3r \int d^3r' \Delta^*(r, r') \hat{\psi}_{\uparrow}(r) \hat{\psi}_{\downarrow}(r') + H.c. \right]. \]

where \( v(r) \) and \( \Delta(r, r') \) are an external potential and an anomalous pair potential respectively. The pairing interaction \( w \) in the particular BCS case satisfies \( w(r'_1, r_1, r_2, r'_2) = w(r'_1 - r_1, r_2 - r'_2) \). The normal and anomalous densities, \( n(r) \) and \( \chi(r, r') \), are defined as

\[ n(r) = \sum_{\sigma} \langle \hat{\psi}_{\sigma}^\dagger(r) \hat{\psi}_{\sigma}(r) \rangle, \]

\[ \chi(r, r') = \langle \hat{\psi}_{\uparrow}(r) \hat{\psi}_{\downarrow}(r') \rangle. \]

The Hohenberg-Kohn theorem for superconductors says that, at each temperature \( \theta = 1/\beta \), the normal and anomalous densities, \( n(r) \) and \( \chi(r, r') \), determine uniquely the density operator \( \hat{\rho} = e^{-\beta \hat{H}_{v,\Delta}}/Tr e^{-\beta \hat{H}_{v,\Delta}} \) which minimizes the thermodynamic potential, \( \Omega_{v,\Delta}[\hat{\rho}] \), given by

\[ \Omega_{v,\Delta}[\hat{\rho}] = Tr \{ \hat{H}_{v,\Delta} + \theta \hat{\rho} \ln \hat{\rho} \}. \]

Furthermore, the thermodynamic potential can be expressed in terms of the densities and potentials by involving a universal functional of the densities, \( F[n, \chi] \), as follows

\[ \Omega_{v,\Delta}[n, \chi] = F[n, \chi] + \int d^3r v(r)n(r) \]

\[ - \int d^3rd^3r' [\Delta^*(r, r')\chi(r, r') + H.c.] \]

The universal functional contains the exchange-correlation (xc) free-energy functional, \( F_{xc}[n, \chi] \), as below

\[ F[n, \chi] = T_s[n, \chi] - \delta S_s[n, \chi] - \mu N \]

\[ + \frac{1}{2} \int d^3r d^3r' \frac{n(r)n(r')}{|r-r'|} \]

\[ - \int d^3r_1 d^3r'_1 d^3r_2 d^3r'_2 \chi^*(r_1, r'_1) \]

\[ \times w(r'_1, r_1, r_2, r'_2)\chi^*(r_2, r'_2) + F_{xc}[n, \chi], \]

where \( T_s[n, \chi] \) and \( S_s[n, \chi] \) are the kinetic energy and the entropy of a noninteracting system with the noninteracting potentials, \( v_s \) and \( \Delta_s \), such that the densities \( n \) and \( \chi \) are equal to those of the noninteracting system. In the above formula, \( \mu \) is the chemical potential.

The noninteracting potentials, \( v_s \) and \( \Delta_s \), consist of the external potentials, \( v_0 \) and \( \Delta_0 \), and Hartree potentials, and the exchange-correlation potentials, \( v_{xc} \) and \( \Delta_{xc} \), as follows

\[ v_s[n, \chi](r) = v_0(r) + \int d^3r' \frac{n(r')}{|r-r'|} + v_{xc}[n, \chi](r), \]

\[ \Delta_s[n, \chi](r, r') = \Delta_0(r, r') + \int d^3r' \frac{\chi(r, r')}{|r-r'|} + \Delta_{xc}[n, \chi](r, r'). \]

The exchange-correlation potentials, \( v_{xc} \) and \( \Delta_{xc} \), are defined as the derivatives of the xc functional, \( F_{xc}[n, \chi] \), with respect to the densities, \( n \) and \( \chi \), correspondingly as below

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

\[ \Delta_{xc}[n, \chi](r, r') = -\frac{\delta F_{xc}[n, \chi]}{\delta \chi(r, r')}. \]

The densities, \( n \) and \( \chi \), are defined as functions of the amplitudes \( u_i(r) \) and \( v_i(r) \) as

\[ n(r) = 2 \sum_i \left[ |u_i(r)|^2 f_{\beta,i} + |v_i(r)|^2 (1 - f_{\beta,i}) \right], \]

\[ \chi(r, r') = \sum_i \left[ v_i^*(r')u_i(r)(1 - f_{\beta,i}) - v_i^*(r)u_i(r')f_{\beta,i} \right]. \]
with the Fermi distribution function \( f_{\beta, i} = 1 + \exp(\beta E_i) \).

At this point, one could guess the densities, \( n \) and \( \chi \), and find the potentials, \( v_{xc} \) and \( \Delta_{xc} \), and solve the KS-BdG equations, and find new densities etc. Further for practical reasons, as we already mentioned at the begin of this Section, one can make two approximations which we will discuss now.

10. The energy scales for the electronic energies and the superconducting energy gap differ by orders of magnitude. Therefore, the KS-BdG equations can be *decoupled* into the Kohn-Sham equation and the gap equation. This approximation was introduced to the SCDF in Ref. [15].

It holds within the **decoupling approximation** that:

(a) the amplitudes \( u_i(r) \) and \( v_i(r) \) can be written in a form

\[
u_i(r) \approx u_i \varphi_i(r) ; \quad v_i(r) \approx v_i \varphi_i(r),
\]

(b) the eigenvalues in Eqs. (8) and (9) are defined by

\[
E_i = \pm \sqrt{\xi_i^2 + |\Delta_i|}
\]

where \( \xi_i = \varepsilon_i - \mu \)

(c) the coefficients \( u_i \) and \( v_i \) are given by

\[
\begin{align*}
u_i &= \frac{1}{\sqrt{2}} \text{sgn}(E_i) e^{i\phi_i} \sqrt{1 + \frac{\xi_i}{E_i}}, \\
v_i &= \frac{1}{\sqrt{2}} \sqrt{1 - \frac{\xi_i}{E_i}},
\end{align*}
\]

and the phase factor \( \phi_i \) is defined by

\[
ee^{i\phi_i} = \frac{\Delta_i}{|\Delta_i|}.
\]

(d) the matrix elements \( \Delta_i \) are defined as

\[
\Delta_i = \int d^3r \int d^3r' \varphi_i^*(r) \Delta_{xc}(r, r') \varphi_i(r'),
\]

and the normal and anomalous densities read respectively

\[
\begin{align*}
n(r) &= \sum_i \left( 1 - \frac{\xi_i}{E_i} \right) \tanh \left( \frac{\beta E_i}{2} \right) |\varphi_i(r)|^2, \\
\chi(r, r') &= \frac{1}{2} \sum_i \frac{\Delta_i}{E_i} \tanh \left( \frac{\beta E_i}{2} \right) \varphi_i^*(r) \varphi_i(r').
\end{align*}
\]

11. The decoupling of the two energy scales yields a transformation of the KS-BdG equations into the ordinary Kohn-Sham equation

\[
\left[ \nabla^2 + v_s[n, \chi](r) - \mu \right] \varphi_i(r) = \varepsilon_i \varphi_i(r),
\]

and the gap equation

\[
\Delta_i = \Delta_{xc,i} |\mu, \Delta_i|.
\]

The Eq. (20) stems from including Eqs. (22) and (24) into Eq. (11), and using the potential given by formula (11) in Eq. (21).

12. In vicinity of \( T_c \), the gap function is vanishing, therefore, it can be *linearized* in \( \Delta_i \).

The above twelve steps lead to the gap equation which can be expressed in the form

\[
\Delta_i = -\frac{1}{2} \sum_j M_{Hxc,ij}[\mu] \tanh \left( \frac{\beta \xi_j}{2} \right) \Delta_j,
\]

\[
M_{Hxc,ij}[\mu] = -\frac{\delta \Delta_{Hxc,i}}{\delta \chi_j},
\]

where \( \Delta_{Hxc,i} \) is defined by Eq. (13).

In other way, Eq. (27) can be written as

\[
\Delta_i = -Z_i[\mu] \Delta_i - \frac{1}{2} \sum_j K_{ij}[\mu] \tanh \left( \frac{\beta \xi_j}{2} \right) \Delta_j.
\]

\( K_{ij} \) and \( Z_i \) are the functionals only of the chemical potential in the case when the gap equation is linearized. The above gap equation will be solved later in this work. The explicit form of the kernel \( K_{ij} \) and the norm \( Z_i \) will be given in Section 6.

Since the gap function contains the exchange-correlation part defined by Eq. (13), we will focus on the construction of the exchange-correlation free-energy functional, \( F_{xc} \), in the following Section.

### 3 Exchange-correlation functional, \( F_{xc}[n, \chi] \)

The derivation of the exchange-correlation energy \( F_{xc} \), by making use of the *perturbative expansion of the thermodynamic potential*, was given in Ref. [12]. For the purpose of inclusion the spin interactions, we will briefly draw a skeleton of this derivation here.

First, one can notice from Eqs. (5) and (6) that

\[
F_{xc} = \Omega - \Omega_s + \int d^3r \left[ v_H(r) + v_{xc}(r) \right] n(r)
\]

\[
- \int d^3r \int d^3r' \left[ \Lambda_{xc}(r, r') \chi(r, r') + \Delta_{xc}(r, r') \chi^*(r, r') \right]
\]

\[
- \frac{1}{2} \int d^3r \int d^3r' \frac{n(r)n(r')}{|r - r'|}.
\]

Then, we take the coupling constant integration formula which reads

\[
\Omega - \Omega_s = \int_0^1 \frac{d\lambda}{\lambda} \langle \lambda \hat{H}_1 \rangle,
\]

where \( \lambda \) is the coupling constant, and the perturbation Hamiltonian \( \hat{H}_1 \) satisfies \( \hat{H} = \hat{H}_s + \lambda \hat{H}_1 \) with the interacting and noninteracting Hamiltonians, \( \hat{H} \) and \( \hat{H}_s \), respectively. The Hamiltonian \( \hat{H}_1 \) contains the difference between the exact Coulomb interaction and the exchange-correlation potentials, the electron-phonon interaction, the
the field operator, \( \hat{1} \). This derivation starts from some algebra, at the relation

\[
\Omega = \int d^3 r \left[ \psi_H(\mathbf{r}) + \psi_{xc}(\mathbf{r}) \right] n^{\lambda}(\mathbf{r}) - \lambda \int d^3 r \left[ v_H(\mathbf{r}) + v_{xc}(\mathbf{r}) \right] n^{\lambda}(\mathbf{r})
\]

which we can plug into the Eq. \( 41 \) for the exchange-correlation functional, \( F_{xc}[n,\chi] \).

As for the first-order selfenergy, \( \Sigma_{\sigma\sigma'} \), for the nonmagnetic systems with the potential \( v(\mathbf{r},\mathbf{r}') \), this energy is defined as

\[
\Sigma(\mathbf{r},\mathbf{r}') = -v(\mathbf{r},\mathbf{r}') \, \tau_3 \tilde{G}(\mathbf{r},\mathbf{r}') \tau_3,
\]

and \( \tau_3 \) is one of the Pauli matrices:

\[
\tau_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau_2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix},
\]

\[
\tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \tau_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.
\]

For the magnetic systems, the matrix \( \tau_3 \) in the each vertex of Feynman diagrams for the selfenergy with the Coulomb and phonon interactions has to be replaced with the matrix \( \tau_0 \tau_3 \).

In this Section, we sketched main steps to be done for finding a general form of the \( F_{xc}[n,\chi] \) functional for a superconductor. The final formula involves the self-energy which will be evaluated in detail for the Coulomb and electron-phonon interactions in the next Section and for the paramagnons in Section 5.

### 4 Coulomb and electron-phonon interactions in \( F_{xc}[n,\chi] \)

The derivation of \( F_{xc} \) for the Coulomb and phonon interactions is given in detail in Refs. \[4,13\]. Here, we report this derivation starting with the interactions in the self-energy (in Eq. \( 42 \)) defined by

\[
v^{el}(\mathbf{r},\mathbf{r}') = \frac{1}{|\mathbf{r} - \mathbf{r}'|},
\]

\[
v^{ph}(\mathbf{r},\mathbf{r}') = V_{\lambda q}(\mathbf{r}) D_{\lambda q}(\tau - \tau') V_{\lambda q}(\mathbf{r}'),
\]

where \( V_{\lambda q} \) is the electron-phonon interaction vertex and \( D_{\lambda q} \) is the phonon Green’s function defined as

\[
D_{\lambda q}(\tau, \tau') = \langle \hat{T}_{\lambda q}(\mathbf{r}) \hat{T}^\dagger_{\lambda q}(\mathbf{r}) \rangle,
\]

with \( \hat{T}_{\lambda q} = b_{\lambda q} + b_{\lambda -q}^\dagger \), and \( b_{\lambda q}^\dagger \) (\( b_{\lambda q} \)) being the phonon creation (annihilation) operators.

Let us have a look now at the expression \[9 \] for \( F_{xc} \) and the definitions of the Nambu Green’s function and selfenergy given by Eqs. \[11 \] and \[12 \] respectively. The
The formulas given below were derived from the definitions and entering Eq. (29), is proportional to
\[ G_{\uparrow \uparrow}G_{\uparrow \uparrow} - F_{\uparrow \downarrow}F_{\uparrow \downarrow} = G_{\uparrow \downarrow}G_{\uparrow \downarrow} + F_{\uparrow \downarrow}F_{\uparrow \downarrow} \]  
(46)
and the corresponding terms with the opposite spins. The above terms appear for both the Coulomb and electron-phonon interactions, and later will lead to the opposite signs in the kernel \( K_{ij} \) and the norm \( Z_i \) of the gap equation. Just mentioned difference in sign, in the first order terms of the total energy with the normal and anomalous Green’s functions, stems from the factor of \((-1)\) which one has to associate with the each loop of anomalous Green’s functions.

In order to evaluate further \( F_{xc} \), we bring here the explicit expressions for the noninteracting propagators. The formulas given below were derived from the definitions assuming the decoupling approximation, i.e. Eqs. (10); the Kohn-Sham orbitals \( \varphi_k(r) \) were chosen to those of a homogeneous gas \( (w_n \) are the odd Matsubara frequencies)
\[ G_{\sigma \sigma'}^{\sigma'}(k, w_n) = \delta_{\sigma, \sigma'} \times \left[ \frac{|u_k|^2}{i \omega_n - E_k} + \frac{|v_k|^2}{i \omega_n + E_k} \right], \]  
(47)
\[ F_{\sigma \sigma'}^{\sigma}(k; w_n) = \delta_{\sigma, -\sigma'} sgn(\sigma') \times u_k v_k \left( \frac{1}{i \omega_n + E_k} - \frac{1}{i \omega_n - E_k} \right), \]  
(48)
\[ F_{\sigma \sigma'}^{\sigma}(k; w_n) = \delta_{\sigma, -\sigma'} sgn(\sigma) \times u_k v_k \left( \frac{1}{i \omega_n + E_k} - \frac{1}{i \omega_n - E_k} \right). \]  
(49)

Now, we will combine Eqs. (29) and (41), for the \( F_{xc} \) and \( \Omega - \Delta \) respectively, with a definition of the Nambu Green’s function, Eq. (41), and an expression for the self-energy, Eq. (12). As for the noninteracting Green’s functions, we use those obtained within the decoupling approximation, i.e. Eqs. (10). This way, one arrives to formulas for the xc energy, stemming from the normal and anomalous loops, which we write here. The “normal” and “anomalous” terms of \( F_{xc} \) for the electronic contributions, \( F_{xc}^{el,1} \) and \( F_{xc}^{el,2} \), are as follows
\[ F_{xc}^{el,1} = -\frac{1}{4} \sum_{kk'} \left( 1 - \frac{\xi_k}{E_k} \right) v(k, k') \left( 1 - \frac{\xi_{k'}}{E_{k'}} \right) \times \tanh \left( \frac{\beta}{2} E_k \right) \tanh \left( \frac{\beta}{2} E_{k'} \right), \]  
(50)
\[ F_{xc}^{el,2} = \frac{1}{4} \sum_{kk'} v(k, k') \frac{\Delta_{k}^2}{E_k} \frac{\Delta_{k'}^2}{E_{k'}} \times \tanh \left( \frac{\beta}{2} E_k \right) \tanh \left( \frac{\beta}{2} E_{k'} \right), \]  
(51)
and the electron-phonon terms, with the normal and anomalous loops, \( F_{xc}^{ph,1} \) and \( F_{xc}^{ph,2} \), respectively are given below
\[ F_{xc}^{ph,1} = -\frac{1}{2} \sum_{kk'} \int d\Omega \alpha^2 F(\Omega) \times \left[ \left( 1 + \frac{\xi_k \xi_{k'}}{E_k E_{k'}} \right) I(E_k, E_{k'}, \Omega) + \left( 1 - \frac{\xi_k \xi_{k'}}{E_k E_{k'}} \right) I(E_k, -E_{k'}, \Omega) \right], \]  
(52)
\[ F_{xc}^{ph,2} = \frac{1}{2} \sum_{kk'} \int d\Omega \alpha^2 F(\Omega) \Delta_k \Delta_{k'} \frac{\Delta_k \Delta_{k'}}{E_k E_{k'}} \times \left[ I(E_k, E_{k'}, \Omega) - I(E_k, -E_{k'}, \Omega) \right]. \]  
(53)
The function \( I(E_k, E_{k'}, \Omega) \) is defined as
\[ I(E_k, E_{k'}, \Omega) = \frac{1}{\beta^2} \sum_{\omega \omega'} \frac{1}{\omega_1 - E_k} \frac{1}{i \omega_2 - E_{k'}} - \frac{2\Omega}{(\omega_1 - \omega_2)^2 + \Omega^2}. \]  
(54)
For the completeness, we give the definitions:
\[ v(k, k') = \int d^3 r d^3 r' \varphi^*_k(r) \varphi_{k'}(r'), \]  
(55)
\[ g_{kk'+q}^{\lambda q} = \int d^3 r \varphi^*_k(r) V_{\lambda q} \varphi_{k+q}(r), \]  
(56)
\[ \alpha^2 F(\Omega) = \frac{1}{N(\varepsilon_F)} \sum_{k} \sum_{\lambda q} \frac{|g_{kk'+q}^{\lambda q}|^2 \delta(\Omega - \omega_{\lambda q})}{\lambda q} \]  
(57)
where \( \omega_{\lambda q} \) is the phonon frequency and \( N(\varepsilon_F) \) is the density of states.

Using the formulas (50) and (51), one is ready to derive the exchange-correlation potential defined by Eq. (13). This derivation can be performed with the help of the chain rule as follows
\[ \Delta_{xc,i} = -\frac{\delta F_{xc}}{\delta \mu} \frac{\delta \mu}{\delta \chi_i^*} - \sum_j \left[ \frac{\delta F_{xc}}{\delta \Delta_j} \frac{\delta |\Delta_j|^2}{\delta \chi_i^*} \right]. \]  
(58)
Further evaluation of the above expression is given in detail in Refs. (12). In this work, we give the final formula for \( \Delta_{xc,i} \) which involves the phonon and paramagnon spectral functions and can be implemented in a straightforward way. We will give the details of implementation in Section 5.

At this point, we arrived to the explicit expressions for \( F_{xc} \) with the electronic and phononic parameters such as: the chemical potential \( \mu \), the density of states \( N(\varepsilon_F) \),
the single particle energies $\varepsilon_k$, and the Eliashberg function $\alpha^2F(\Omega)$. Now, we are ready to introduce the spin fluctuations into the discussed formalism, and we will this in the following Section.

5 Paramagnons in $F_{xc}[n, \chi]$

We will introduce the transverse spin-fluctuations to the total energy within the SCDF. For the simplicity, we will assume the singlet pairing and the s-wave symmetry of the gap function. The extension to triplet superconductors could be done following the work by Capelle et al. [16,20]. For the case of magnetic superconductors, one should take also into account a correction for the Zeeman effect, i.e. the spin gap. As for the paring potentials with the higher angular-momentum, one cannot average spherically the angular part of the interaction in the RPA formula for the paramagnon susceptibility, which formula will be used later in this Section.

Here, we start with the Nambu Green’s function for the superconductors with magnetic interactions included into the description. This matrix is now 4×4 dimensional and reads

$$\hat{G}(r, r'; \tau') = -\langle \hat{T} \hat{\psi}(r, \tau) \otimes \hat{\psi}^\dagger(r', \tau') \rangle,$$  

with the 4-component field operators (the notation has been chosen according to Maki in Ref. [18] and $x$ denotes the vector $(r, \tau)$)

$$\hat{\psi}(x) = \left( \begin{array}{c} \hat{\psi}_1(x) \\ \hat{\psi}_2(x) \\ \hat{\psi}_3(x) \\ \hat{\psi}_4(x) \end{array} \right), \quad \hat{\psi}^\dagger(x) = \left( \begin{array}{c} \hat{\psi}_1^\dagger(x) \hat{\psi}_2^\dagger(x) \hat{\psi}_3^\dagger(x) \hat{\psi}_4^\dagger(x) \end{array} \right).$$  

(60)

The first-order selfenergy with the spin dependent interaction $v^{\mu\nu}$, where $\mu$ and $\nu$ denote the cartesian components of the spin orientations of two interacting electrons, is given by

$$\Sigma(r, r'; \tau') = -v^{\mu\nu}(r, r'; \tau') \tilde{\alpha}_\mu \hat{G}(r, r'; \tau') \tilde{\alpha}_\nu,$$  

$v^{\mu\nu}(r, r'; \tau') = I_{ex}(r)D^{\mu\nu}(\tau - \tau')I_{ex}(r'),$  

(61)

(62)

The quantity $I_{ex}$ is the spin exchange interaction, and $D^{\mu\nu}$ is the spin Green’s function. The matrix $\tilde{\alpha}_\mu$ is defined as

$$\tilde{\alpha}_\mu = \left( \begin{array}{c} \sigma_\mu^x \\ 0 \\ 0 \\ -\sigma_\mu^y \end{array} \right),$$  

(63)

where $\sigma_\mu^x$ denotes a matrix transposed to the Pauli matrix $\sigma_\mu$ (see Ref. [19]).

For the transverse spin fluctuations, the $\alpha$-matrix, given by formula [18], involves the Pauli matrices $\sigma^+ = \frac{1}{2}(\sigma_x + i\sigma_y)$; explicitly

$$\sigma^+ = \left( \begin{array}{cc} 0 & 1 \\ 0 & 0 \end{array} \right), \quad \sigma^- = \left( \begin{array}{cc} 0 & 0 \\ 1 & 0 \end{array} \right).$$

Evaluation of the selfenergy with paramagnons, according to Eqs. (61,63), yields a very sparse 4×4-matrix which reads

$$\Sigma(r, r'; \tau') = -v^{+-}(r, \tau' \tau') \left( \begin{array}{cccc} G_{++}(r, r'; \tau') & 0 & 0 & 0 \\ 0 & G_{++}(r, r'; \tau') & 0 & 0 \\ 0 & 0 & G_{++}(r, r'; \tau') & 0 \\ 0 & 0 & 0 & G_{++}(r, r'; \tau') \end{array} \right),$$  

(64)

where $G_{++} = -G_{++}$.

Now, if we go back to the previous section and look again at the (1,1)-element of the ($\Sigma G$)-matrix, we will remind to us that for the Coulomb and electron-phonon interactions, the total energy is proportional to the expression [16]. For the magnetic interactions, however, for which the Nambu Green’s function has been defined by Eq. (64), and the selfenergy has been given by Eq. (64), the total energy is proportional to

$$G_{++}G_{++} - F_{++}F_{++} = G_{++}G_{++} - F_{++}F_{++}.$$  

(65)

The above expression differs from relation [16] by signum in front of the anomalous Green’s functions. This difference will show up in the kernel $K_\lambda$ and the norm $Z_i$ of the gap equation such that, both the phonon and paramagnon spectral functions enter the kernel with different signum (originating from the anomalous loop of Green’s functions) and the norm with the same signum (originating from the normal loop).

To proceed further with the evaluation of the xc-free energy, $F_{xc}$, we write explicitly the spin-fluctuation Green’s function, $D^{\mu\nu}(\tau - \tau')$, used in Eq. (62). In the case of paramagnons, $D^{\mu\nu}(\tau - \tau')$ is the transverse spin susceptibility, $\chi^{+-}$, defined as

$$\chi^{+-}(r, r'; \tau - \tau') = \langle \hat{T} \hat{S}^-(r, \tau) \hat{S}^+(r', \tau') \rangle,$$  

(66)

with the operators increasing and lowering spin which are defined respectively as

$$\hat{S}^+(r, \tau) = \hat{\psi}_1^\dagger(r, \tau) \hat{\psi}_1(r, \tau),$$  

$$\hat{S}^-(r, \tau) = \hat{\psi}_1^\dagger(r, \tau) \hat{\psi}_1(r, \tau).$$  

(67)

(68)

For the conduction band, we can use a model of the homogeneous electron gas with the fluctuations treated on the level of the random phase approximation. The Fourier transform of the RPA-“dressed” paramagnon propagator is

$$\chi^{+-}(q, \nu_n) = \frac{\chi^0(q, \nu_n)}{1 - I_{ex} \chi^0(q, \nu_n)},$$  

(69)

with the Pauli susceptibility $\chi^0$ and the even Matsubara frequencies $\nu_n$. 

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It is convenient to introduce the spectral representation
\[ \chi^+(q,\nu_n) = -\int_0^\infty \frac{d\Omega}{\pi} D^0(\Omega,\nu_n) \Im m \chi^+(q,\Omega), \]
\[ D^0(\Omega,\nu_n) = -\frac{2\Omega}{k_n^2 + \Omega^2}, \]
and the momentum averaged paramagnon spectral function
\[ P(\Omega) = N(\varepsilon_F) \int_0^{2k_F} dq \frac{q}{2k_F^2} \]
\[ \times |I(q)|^2 \left[ -\frac{1}{\pi} \Im m \chi^+(q,\Omega) \right]. \]

We assume that the interaction function, \( I(q) \), is the momentum independent quantity \( I_{ex} \), which can be calculated in a way given for instance in Ref. \[10\].

Therefore, for the systems with the electron-paramagnon interactions, the exchange-correlation free energy is given by
\[ F^{sf,1}_{ex} = -\frac{1}{2} \sum_{kk'} \int d\Omega P(\Omega) \]
\[ \times \left[ \left( 1 + \frac{\xi_k\xi_{k'}}{E_kE_{k'}} \right) I(E_k,E_{k'},\Omega) \right. \]
\[ \left. + \left( 1 - \frac{\xi_k\xi_{k'}}{E_kE_{k'}} \right) I(E_k,-E_{k'},\Omega) \right], \]
\[ F^{sf,2}_{ex} = -\frac{1}{2} \sum_{kk'} \int d\Omega P(\Omega) \frac{A_k-A_{k'}}{E_kE_{k'}} \]
\[ \times \left[ I(E_k,E_{k'},\Omega) - I(E_k,-E_{k'},\Omega) \right], \]
where the function \( I(E_k,E_{k'},\Omega) \) is defined by Eq. \[54\]. The explicit formula for the paramagnon spectral function, \( P(\Omega) \), within the RFA is given for instance in Refs. \[8,19,10\].

6 Gap equation with paramagnons and implementation details

At this point, when we have completed the derivation of all components of the exchange-correlation free energy: the Coulomb part - Eqs. \[55,61\], the phonon part - Eqs. \[52,53\], and the spin-fluctuation part - Eqs. \[63,64\], we can write explicitly the gap equation given by Eqs. \[56,58\].

The \( M_{ij} \)-matrix of the linearized equation \[28\] is the following function of the kernel \( K_{ij} \) and the norm \( Z_i \)
\[ M_{ij} = -\frac{1}{2} K_{ij} \left( \Delta = 0 \right) \]
\[ = -\frac{1}{2} \frac{K_{ij}}{1 - Z_i \left( \Delta = 0 \right)}. \]

The nondiagonal part of the \( M_{ij} \)-matrix is given by
\[ K_{ij} = K_{ij}^{el} + K_{ij}^{ph+sf}, \]
where the electronic part is defined by
\[ K_{ij}^{el} = w_{ij}, \]
\[ w_{ij} = \frac{2\pi}{k_i k_j} \log \left( \frac{(k_i + k_j)^2 + k_{ TF}^2}{(k_i - k_j)^2 + k_{ TF}^2} \right). \]

The Coulomb interaction \( w_{ij} \) has been spherically averaged over the angular coordinates since, as we said before, we assumed the \( s \)-wave pairing. The electron correlations are taken into account by the Thomas-Fermi screening constant, \( k_{ TF} \), and \( k_i \) is an absolute value of the reciprocal vector.

The electron-phonon and -paramagnon interaction diagonal part of the \( M_{ij} \)-matrix is given by
\[ K_{ij}^{ph+sf} = \frac{2}{\tanh(\beta \xi_i/2) \tanh(\beta \xi_j/2)} \]
\[ \times \int d\Omega \left[ a^2 F(\Omega) - P(\Omega) \right] \]
\[ \times \left[ I(\xi_i,\xi_j,\Omega) - I(\xi_i,-\xi_j,\Omega) \right]. \]

The diagonal part of the \( M_{ij} \)-matrix is
\[ Z_i = Z_i^{el} + Z_i^{ph+sf}, \]
where the purely electronic part is
\[ Z_i^{el} = -\frac{1}{2\xi_i} \left\{ \sum_j w_{ij} \left[ 1 - \tanh(\beta \xi_j/2) \right] \right. \]
\[ - \frac{\beta w_{ij}^2}{\sum_k \cosh^2(\beta \xi_k/2)} \left[ 1 - \tanh(\beta \xi_i/2) \right] \right\}, \]
and the phononic and paramagnon part is
\[ Z_i^{ph+sf} = \frac{-4\pi}{\tanh(\beta \xi_i/2) \beta} \int d\Omega \left[ a^2 F(\Omega) + P(\Omega) \right] \]
\[ \times \sum_{\omega_2} \omega_2 \text{sgn}(\omega_2) \left[ Z_{i,\text{sym}}^{ph+sf} + Z_{i,\text{asym}}^{ph+sf} \right], \]
\[ Z_{i,\text{sym}}^{ph+sf} = \left[ n_{\beta}(\Omega) + f_{\beta}(\xi_i) \right] \frac{2(\xi_i + \Omega)}{[\omega_2^2 + (\xi_i + \Omega)^2]}, \]
\[ + \left[ n_{\beta}(\Omega) + f_{\beta}(\xi_i) \right] \frac{2(\xi_i - \Omega)}{[\omega_2^2 + (\xi_i - \Omega)^2]}. \]

Functions \( f_{\beta} \) and \( n_{\beta} \) are the Fermi-Dirac and Bose-Einstein distribution functions respectively.

For the electronic part of the norm, i.e. \( Z_i^{el} \), we used the zero temperature approximation given in Refs. \[14,10\]. This approximation can be justified by the fact that the critical temperatures of simple metals, which we calculate in this work, are very low. The above simplification is done for sake of a numerical convenience since there are many singularities in the formula \[81\].

The subscripts "sym" and "asym" mean the symmetric and antisymmetric part of \( Z_i \) with respect to the electron-phonon coupling elements \( g_{kk'kq} \). The electron-paramagnon
interaction constant, $I(q)$, has been also averaged in $q$ leading to $I_{ex}$. The antisymmetric part $Z_{i, asym}^{ph + sf}$ is omitted in our calculations according to the reasons discussed in Refs. [10] and in our previous work [11]. Therefore, we do not give the expression for $Z_{i, asym}^{ph + sf}$ in this work.

7 Critical temperatures of simple metals

In the following two subsections, we report the critical temperatures obtained by solving the SCFDT gap equation with spin fluctuations included. We compare these results with the results without spin fluctuations and results from the Eliashberg theory. First, we calculate parameters of the gap equation for several simple metals: V, Mo, Ta, and Pd (fcc and bcc) at ambient pressure. At the end, we complete our previous results for Nb under pressure [10] reporting $T_c$ obtained within the SCFDT with the paramagnons included.

The electronic structures, the densities of states (DOS) and the electron-phonon coupling constants and the phonon and magnon spectral functions for studied metals were calculated within the local density approximation (LDA). We used the pseudopotential plane wave codes pwscf [21] and espressivo [22]. The phonons and electron-phonon couplings were obtained from the density functional perturbation theory (DFPT) [23]. Since the calculation of the spectral function $\alpha^2 F$ is very time consuming, we used the ultrasoft pseudopotentials (US PPs) [24]. The kinetic energy cut-offs for the wavefunctions and densities were 45 Ry and 270 Ry respectively in order to reproduce well all features of the phonon dispersions especially for the low frequency phonons (see Ref. [10]). The metallic broadening at the Fermi energy [25] was assumed at 0.03 Ry. We used the Monkhorst-Pack mesh [26] of (64,64,64)-points for the DOS calculations, (16,16,16)-points for the self-consistent calculation of the electron-phonon-coupling matrix elements for the each phonon, the mesh of (8,8,8)-points to fit the phonon dispersions, and the fit from (16,16,16) into (64,64,64) mesh-points to perform the integrands with the double-delta function present in the definition of the electron-phonon coupling constant, $\lambda^{ph}$, and the spectral function, $\alpha^2 F(\omega)$.

The spin-exchange interaction containst, $I_{ex}$, for metals at ambient pressure were taken from the work by Singalas et al. [27], and further we used them for the calculation of the spectral functions, $P(\omega)$, and the electron-paramagnon coupling constant, $\lambda^{sf}$. For niobium under pressure, we used $I_{ex}$ and $P(\omega)$ calculated in our previous work [10].

All electronic parameters and the phonon and magnon spectral functions were assumed to be the same for the normal and superconducting state. The accuracy of functions $\alpha^2 F(\omega)$ and $P(\omega)$ is very important for an exact estimation of the critical temperature. The electron-phonon spectral function, very time consuming for calculations, contains all the specific information about the studied system. In contrast to $\alpha^2 F(\omega)$, the approximation which we used for the paramagnon spectral function, to avoid calculation of this quantity from the time-dependent density functional theory, is insufficient. We made the assumption of the homogeneous electron gas for the spin susceptibility and the only spin-dependent quantity which we calculated specifically for a given metal was the exchange constant. The calculation of this constant, i.e. $I_{ex}$, is very difficult and obtained results have a large error due to their very small values and necessity to calculate a response function to small magnetizations applied to the system. Therefore, as we will see below, the obtained critical temperatures are not always very close to the experimental ones. Further development should be directed into more accurate calculation of the spectral functions, especially $P(\omega)$.

7.1 Transition metals at ambient pressure

In TABLE II we report the critical temperatures and parameters which enter the gap equation calculated by means of the Eliashberg theory and the SCFDT for a few simple metals: vanadium, molybdenum and tantalum in bcc lattice structure and palladium in fcc and bcc
structures. Our calculated densities of states, $N(\varepsilon_F)$, and electron-phonon coupling constants, $\lambda^{ph}$, are in a good agreement with previous calculations by Savrasov et al.\cite{28}. The Eliashberg functions calculated within the DFPT are presented in FIG. 1. The Coulomb parameter, $\mu^*$, was obtained from the Bennemann-Garland formula\cite{29}, which employs the density of states. The spin exchange constant, $I_{ex}$, taken from Ref.\cite{27}, has been used to obtain the paramagnon spectral function, $P(\omega)$, which we draw in FIG. 2.

As for the critical temperatures, for tantalum, the SCDFT result is in a very small relative error, defined in TABLE 1 of 3% with respect to the experimental data\cite{30}. While, the Eliashberg result with spin fluctuations included is in the error of 81%. For molibdenium, $T_c$ from the Eliashberg gap equation is smaller than the experimental one, even without the paramagnon effect. But the absolute error of all calculated temperatures for Mo is smaller than 1 K. Palladium in both structures fcc and bcc is nonsuperconducting and the SCDFT reproduces well this result. In contrast to the SCDFT result, from the Eliashberg theory we obtained superconductivity for Pd in the bcc structure with a very small $T_c$.

Usually, the critical temperatures from the SCDFT are lower than temperatures from the Eliashberg theory. In some cases, however, the SCDFT temperatures are higher. This situation is for vanadium and molibdenium. Especially for vanadium, $T_c$ from the SCDFT gap equation is about 2 K higher than the experimental data\cite{30}, even after inclusion of spin fluctuations. This fact may indicate that, either the spin exchange constant, $I_{ex}$, was underestimated, or a contribution of the asymmetric part of the phononic term in the SCDFT gap equation is quite large. As we know from results reported in Refs.\cite{5,10}, if we neglect the asymmetric part in the electron-phonon-coupling matrix elements by taking the $\alpha^2F(\omega)$ averaged at the Fermi level, the critical temperatures are higher (see the discussion in Section 4). The last approximation, however, has to be done if we do not evaluate formulas with the $g_{k,k+q}$ elements explicitly.

In general, the critical temperatures obtained from the SCDFT are in a good agreement with the measured temperatures\cite{30}, and the effect of paramagnons improves the result considerable for many simple metals.

### 7.2 Niobium under pressure

In TABLE 2 we present critical temperatures and parameters of the gap equation for niobium at eight pressures in the range from -17 GPa up to 80 GPa. The spin exchange constants, $I_{ex}$, have been calculated from first principles in Ref.\cite{10}, and the electron-phonon and electron-magnon spectral functions for Nb have been presented also in that work.

Here, we complete our previous results by reporting the effect of paramagnons on $T_c$ calculated from the SCDFT. After the inclusion of spin fluctuations, the critical temperatures obtained from the SCDFT are closer to the experimental $T_c$’s for pressures in the range of 0-40 GPa, i.e. pressures between two anomalies measured by Struzhkin et al.\cite{11}. The dependence of the measured critical temperature as a function of pressure is no longer reproduced by our calculations when we take into account paramagnons. At ambient pressure and for higher pressures, paramagnons seem to make the theoretical result worse. The above effect, could be explained by making the observation that, in every case where the exchange constant $I_{ex}$ is large, the theoretical temperature underestimates the measured temperature, and vice versa, for the smallest $I_{ex}$, the critical temperature obtained from the SCDFT is the highest and the error is positive.

Concluding this Subsection, the implementation of paramagnons to the SCDFT generally makes calculated critical temperatures closer to the experimental ones. But our calculated exchange constants, $I_{ex}$, are not sufficiently ac-

### Table 1. Various parameters such as: the crystal symmetry, density of states $N(\varepsilon_F)$ per Ry and per both spins, coupling constants $I_{ex}$ [Ry/both spins], electron-phonon $\lambda^{ph}$, electron-paramagnon $\lambda^{sf}$, and $T_c$ [K] calculated from the Eliashberg theory and the SCDFT with the Coulomb and phonon interactions only (ep) and with spin fluctuations (epsf), the experimental $T_c^{exp}$ (from Ref.\cite{30}), and the ”error” defined as $(T_c^{epsf} - T_c^{exp})/T_c^{exp} [%]$ with $T_c^{epsf}$ calculated within the SCDFT.

| system | $N(\varepsilon_F)$ | $I_{ex}$ | $\lambda^{ph}$ | $\lambda^{sf}$ | $\mu^*$ | Eliashberg | SCDFT | $T_c^{exp}$ | $T_c^{epsf}$ | $\sim T_c^{exp}$ "error" |
|--------|-------------------|---------|----------------|----------------|--------|------------|--------|-------------|--------------|---------------------|
| V bcc  | 24.98 (26.14)     | 0.0218b | 0.91 (1.19°)   | 0.430          | 0.212  | 9.0        | 5.9    | 16.1        | 7.4          | 5.38                | 38                  |
| Mo bcc | 8.81 (8.34°)      | 0.0184b | 0.47 (0.42°)   | 0.024          | 0.198  | 0.8        | 0.7    | 1.5         | 1.4          | 0.92                | 52                  |
| Ta bcc | 18.60 (18.38°)    | 0.0162b | 0.97 (0.86°)   | 0.096          | 0.209  | 8.7        | 8.1    | 5.9         | 4.6          | 4.48                | 3                   |
| Pd fcc | 30.68 (34.14°)    | 0.0230b | 0.35 (0.35°)   | 0.972          | 0.213  | 0.01       | -      | -           | -            | -                   | -                   |
| Pd bcc | 16.60 (18.49°)    | 0.0229b | 0.68 (-)       | 0.167          | 0.208  | 1.3        | 0.8    | -           | -            | -                   | -                   |

\* Values from Ref.\cite{28}.

\* Values from Ref.\cite{27}.

\* Calculated with $I_{ex}$ from Ref.\cite{27}.

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Table 1. Various parameters such as: the crystal symmetry, density of states $N(\varepsilon_F)$ per Ry and per both spins, coupling constants $I_{ex}$ [Ry/both spins], electron-phonon $\lambda^{ph}$, electron-paramagnon $\lambda^{sf}$, and $T_c$ [K] calculated from the Eliashberg theory and the SCDFT with the Coulomb and phonon interactions only (ep) and with spin fluctuations (epsf), the experimental $T_c^{exp}$ (from Ref.\cite{30}), and the ”error” defined as $(T_c^{epsf} - T_c^{exp})/T_c^{exp} [%]$ with $T_c^{epsf}$ calculated within the SCDFT.
SCDFT calculations for T and details of implementation. We assumed singlet and through the decoupling approximation, the gap equation for superconductors. The SCDFT is presented from its foundations, fluctuations to the density functional theory for superconductors.

In the present work, we included the transverse spin fluctuations to the density functional theory for superconductors. The SCDFT is presented from its foundations, through the decoupling approximation, the gap equation and details of implementation. We assumed singlet and s-wave pairing potential; The extension to triplet superconductors could be done following the work by Capelle et al.

Table 2. Results for Nb; applied pressure p [GPa], density of states N(ε_F) per Ry and per both spins, spin exchange integral I_{ex} [Ry/both spins] (from Ref. [10]), coupling constants: electron-phonon λ^{ph}, electron-paramagnon λ^{sf}, and T_c [K] calculated from the Eliashberg theory (with µ =0.21) and SCDFT with Coulomb and phonon interactions only (ep) and with spin fluctuations (epsf). The experimental T^{exp} has been estimated from the picture given in Ref. [11]. Last column shows the "error" of the SCDFT calculations for T^{epsf} defined in TABLE 1.

| p    | N(ε_F)  | I_{ex} | λ^{ph} | λ^{sf} | T^{ep}_c | T^{epsf}_c | ~ T^{exp}_c | "error" |
|------|---------|--------|--------|--------|----------|-----------|------------|---------|
| -16.59 | 22.82  | 0.0211 | 1.91   | 0.28   | 20.3     | 16.7      | 14.4       | 6.2     |   -    |
| -9.45  | 21.60  | 0.0213 | 1.60   | 0.25   | 19.5     | 15.5      | 13.2       | 6.4     |   -    |
| -0.63  | 20.24  | 0.0217 | 1.41   | 0.22   | 18.8     | 14.7      | 12.9       | 7.2     | 9.2    |
| 9.98   | 19.38  | 0.0204 | 1.65   | 0.17   | 19.6     | 15.8      | 13.4       | 9.8     | 10.0   |
| 22.89  | 18.32  | 0.0189 | 1.47   | 0.13   | 19.4     | 16.0      | 13.2       | 11.3    | 9.8    |
| 38.79  | 17.10  | 0.0228 | 1.29   | 0.16   | 18.4     | 14.1      | 12.0       | 10.1    | 9.7    |
| 56.73  | 15.42  | 0.0292 | 1.10   | 0.23   | 16.1     | 10.7      | 10.1       | 8.4     | 9.5    |
| 78.37  | 13.10  | 0.0347 | 0.86   | 0.24   | 13.7     | 7.3       | 8.2        | 7.9     | 8.8    |

8 Summary

In the present work, we included the transverse spin fluctuations to the density functional theory for superconductors. The SCDFT is presented from its foundations, through the decoupling approximation, the gap equation and details of implementation. We assumed singlet and s-wave pairing potential; The extension to triplet superconductors could be done following the work by Capelle et al.

Table 2. Results for Nb; applied pressure p [GPa], density of states N(ε_F) per Ry and per both spins, spin exchange integral I_{ex} [Ry/both spins] (from Ref. [10]), coupling constants: electron-phonon λ^{ph}, electron-paramagnon λ^{sf}, and T_c [K] calculated from the Eliashberg theory (with µ =0.21) and SCDFT with Coulomb and phonon interactions only (ep) and with spin fluctuations (epsf). The experimental T^{exp} has been estimated from the picture given in Ref. [11]. Last column shows the "error" of the SCDFT calculations for T^{epsf} defined in TABLE 1.

| p    | N(ε_F)  | I_{ex} | λ^{ph} | λ^{sf} | T^{ep}_c | T^{epsf}_c | ~ T^{exp}_c | "error" |
|------|---------|--------|--------|--------|----------|-----------|------------|---------|
| -16.59 | 22.82  | 0.0211 | 1.91   | 0.28   | 20.3     | 16.7      | 14.4       | 6.2     |   -    |
| -9.45  | 21.60  | 0.0213 | 1.60   | 0.25   | 19.5     | 15.5      | 13.2       | 6.4     |   -    |
| -0.63  | 20.24  | 0.0217 | 1.41   | 0.22   | 18.8     | 14.7      | 12.9       | 7.2     | 9.2    |
| 9.98   | 19.38  | 0.0204 | 1.65   | 0.17   | 19.6     | 15.8      | 13.4       | 9.8     | 10.0   |
| 22.89  | 18.32  | 0.0189 | 1.47   | 0.13   | 19.4     | 16.0      | 13.2       | 11.3    | 9.8    |
| 38.79  | 17.10  | 0.0228 | 1.29   | 0.16   | 18.4     | 14.1      | 12.0       | 10.1    | 9.7    |
| 56.73  | 15.42  | 0.0292 | 1.10   | 0.23   | 16.1     | 10.7      | 10.1       | 8.4     | 9.5    |
| 78.37  | 13.10  | 0.0347 | 0.86   | 0.24   | 13.7     | 7.3       | 8.2        | 7.9     | 8.8    |

accurate. This fact gives a direction for the future development.

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