

ebmb

Solve multiband ELIASHBERG equations

Outline

This software provides three programs:

1. `ebmb` itself solves the multiband ELIASHBERG equations (Eqs. 1 or 4) on a cut-off imaginary axis and optionally continues the results to the real axis via PADÉ approximants.
A material is defined by nothing but an ELIASHBERG spectral function or, as fallback, an EINSTEIN phonon frequency and intra- and interband electron-phonon couplings, COULOMB pseudo-potentials and, if desired, the band densities of BLOCH states, otherwise assumed to be constant.
2. `critical` finds the critical point via the bisection method varying a parameter of choice. Superconductivity is defined by the kernel of the linearized gap equation (Eq. 5) having an eigenvalue greater than or equal to unity.
3. `tc` finds the critical temperature for each band separately via the bisection method. Superconductivity is defined by the order parameter exceeding a certain threshold. Usually, it is preferable to use `critical`.

Installation

The makefile is designed for the *GNU* or *Intel* Fortran compiler:

```
$ make FC=gfortran FFLAGS=-O3
```

I/O

- Parameters are defined on the command line:

```
$ {program} {key 1}={value 1} {key 2}={value 2} ...
```

The available keys and default values are listed in Table 1.

- Unless `tell=false`, the results are printed to standard output.
- Unless `file=None`, a binary output file is created. For `critical` and `tc` it simply contains one or more double precision floating point numbers, for `ebmb` the format defined in Tables 2 and 3 is used.
- The provided *Python* wrapper functions load the results into *NumPy* arrays:

```
import ebmb
results = ebmb.get({program}, {file}, {replace},
                  {key 1}={value 1}, {key 2}={value 2}, ...)
```

`{replace}` decides whether an existing `{file}` is used or overwritten.

Given a band structure, its discretized domain and $n - 1$ filters, an input file with the density of states resolved for n subdomains is generated like this:

```
from numpy import cos, dot, linspace, pi
DOSfile('dos.in', epsilon=lambda *k: -cos(k).sum() / 2,
        domain=[linspace(-pi, pi, 1000, endpoint=False)] * 2,
        filters=[lambda *k: pi ** 2 / 2 <= dot(k, k) <= pi ** 2])
```

Let $\hbar = k_B = 1$. Fermionic and bosonic MATSUBARA frequencies are defined as $\omega_n = (2n+1)\pi T$ and $\nu_n = 2n\pi T$, respectively. The quantity of interest is the NAMBU self-energy matrix¹

$$\Sigma_i(n) = i\omega_n[1 - Z_i(n)]\mathbf{1} + \underbrace{Z_i(n)\Delta_i(n)}_{\phi_i(n)}\sigma_1 + \chi_i(n)\sigma_3,$$

where the PAULI matrices are defined as usual and i is a band index. Renormalization $Z_i(n)$, order parameter $\phi_i(n)$ and energy shift $\chi_i(n)$ are determined by the ELIASHBERG equations²

$$\begin{aligned} Z_i(n) &= 1 + \frac{T}{\omega_n} \sum_j \sum_{m=0}^{N-1} \int_{-\infty}^{\infty} d\varepsilon \frac{n_j(\varepsilon)}{n_j(\mu_0)} \frac{\omega_m Z_j(m)}{\Theta_j(\varepsilon, m)} \Lambda_{ij}^-(n, m), \\ \phi_i(n) &= T \sum_j \sum_{m=0}^{N-1} \int_{-\infty}^{\infty} d\varepsilon \frac{n_j(\varepsilon)}{n_j(\mu_0)} \frac{\phi_j(m)}{\Theta_j(\varepsilon, m)} [\Lambda_{ij}^+(n, m) - U_{ij}^*(m)], \\ \chi_i(n) &= -T \sum_j \sum_{m=0}^{N-1} \int_{-\infty}^{\infty} d\varepsilon \frac{n_j(\varepsilon)}{n_j(\mu_0)} \frac{\varepsilon - \mu + \chi_j(m)}{\Theta_j(\varepsilon, m)} \Lambda_{ij}^+(n, m), \\ \Theta_i(\varepsilon, n) &= [\omega_n Z_i(n)]^2 + \phi_i^2(n) + [\varepsilon - \mu + \chi_i(n)]^2, \end{aligned} \quad (1)$$

and may then be analytically continued to the real-axis by means of PADÉ approximants.³ The electron-phonon coupling matrices and the rescaled COULOMB pseudo-potential are connected to the corresponding input parameters via

$$\begin{aligned} \Lambda_{ij}^{\pm}(n, m) &= \lambda_{ij}(n - m) \pm \lambda_{ij}(n + m + 1), \quad \lambda_{ij}(n) = \int_0^{\infty} d\omega \frac{2\omega \alpha^2 F_{ij}(\omega)}{\omega^2 + \nu_n^2} \underset{\text{Einstein}}{=} \frac{\lambda_{ij}}{1 + \left[\frac{\nu_n}{\omega_E}\right]^2}, \\ U_{ij}^*(m) &= \begin{cases} 2\mu_{ij}^*(N_C) & \text{for } m < N_C, \\ 0 & \text{otherwise,} \end{cases} \quad \frac{1}{\mu_{ij}^*(N_C)} = \frac{1}{\mu_{ij}^*} + \ln \frac{\omega_E}{\omega_{N_C}} \end{aligned} \quad (2)$$

with the ELIASHBERG spectral function $\alpha^2 F_{ij}(\omega)$. Alternatively, if the band density $n_i(\varepsilon)$ of BLOCH states with energy ε per spin, band and unit cell is given,

$$\frac{1}{\mu_{ij}^*(N_C)} = \frac{1}{\mu_{ij}^*} + \ln \frac{2\omega_E}{D} + \frac{1}{\pi} \sum_i \int_{-\infty}^{\infty} d\varepsilon \frac{n_i(\varepsilon)}{n_i(\mu_0)} \begin{cases} \frac{1}{\varepsilon - \mu_0} \arctan \frac{\varepsilon - \mu_0}{\omega_{N_C}} & \text{for } \varepsilon \neq \mu_0, \\ \frac{1}{\omega_{N_C}} & \text{otherwise,} \end{cases} \quad (3)$$

where D is the electronic bandwidth. μ_0 and μ are the chemical potentials for free and interacting particles. The corresponding occupancy number $n_0, n \in (0, 2)$ is usually conserved:

$$2 \sum_i \int_{-\infty}^{\infty} d\varepsilon \frac{n_i(\varepsilon)}{e^{(\varepsilon - \mu_0)/T} + 1} = n_0 \stackrel{!}{=} n \approx 1 - 4T \sum_i \int_{-\infty}^{\infty} d\varepsilon n_i(\varepsilon) \left[\sum_{n=0}^{N-1} \frac{\varepsilon - \mu + \chi_i(n)}{\Theta_i(\varepsilon, n)} + \frac{\arctan \frac{\varepsilon - \mu}{\omega_N}}{2\pi T} \right].$$

Approximating $n_i(\varepsilon) \approx n_i(\mu_0)$ yields $\chi_i(n) = 0$ and the constant-DOS ELIASHBERG equations

$$\begin{aligned} Z_i(n) &= 1 + \frac{\pi T}{\omega_n} \sum_j \sum_{m=0}^{N-1} \frac{\omega_m}{\sqrt{\omega_m^2 + \Delta_j^2(m)}} \Lambda_{ij}^-(n, m), \\ \Delta_i(n) &= \frac{\pi T}{Z(n)} \sum_j \sum_{m=0}^{N-1} \frac{\Delta_j(m)}{\sqrt{\omega_m^2 + \Delta_j^2(m)}} [\Lambda_{ij}^+(n, m) - U_{ij}^*(m)]. \end{aligned} \quad (4)$$

¹Y. NAMBU, Phys. Rev. **117**, 648 (1960)

²G. M. ELIASHBERG, Soviet Phys. JETP **11**, 696 (1960).

A comprehensive review is given by P. B. ALLEN and B. MITROVIĆ in Solid state physics **37** (1982)

³H. J. VIDBERG and J. W. SERENE, J. Low Temp. Phys. **29**, 179 (1977)

At the critical temperature, $\Delta_i(m)$ is infinitesimal and negligible relative to ω_m . This yields

$$\begin{aligned}\Delta_i(n) &= \sum_j \sum_{m=0}^{N-1} K_{ij}(n, m) \Delta_j(m), \\ K_{ij}(n, m) &= \frac{1}{2m+1} [\Lambda_{ij}^+(n, m) - \delta_{ij} \delta_{nm} D_i^N(n) - U_{ij}^*(m)], \\ D_i^N(n) &= \sum_j \sum_{m=0}^{N-1} \Lambda_{ij}^-(n, m) \stackrel{N=\infty}{=} \sum_j \left[\lambda_{ij} + 2 \sum_{m=1}^n \lambda_{ij}(m) \right].\end{aligned}\tag{5}$$

$Z_i(n)$ is not biased by the cutoff if $D_i^\infty(n)$ is used in place of $D_i^N(n)$ in the kernel $K_{ij}(n, m)$.

For a given scalar $\alpha^2 F(\omega)$, an effective phonon frequency can be calculated in different ways. We follow ALLEN and DYNES,⁴ who define the logarithmic average frequency

$$\omega_{\log} = \exp \left[\frac{2}{\lambda} \int_0^\infty \frac{d\omega}{\omega} \alpha^2 F(\omega) \ln(\omega) \right]$$

and the second-moment average frequency

$$\bar{\omega}_2 = \sqrt{\frac{2}{\lambda} \int_0^\infty d\omega \alpha^2 F(\omega) \omega}.$$

and choose $\bar{\omega}_2$ for ω_E in Eqs. 2 and 3 for rescaling μ^* .

— Acknowledgment —

Parts of the program are inspired by the EPW code⁵ and work of Malte Rösner.

— Contact —

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⁴P. B. ALLEN and R. C. DYNES, Phys. Rev. B **12**, 905 (1975)

⁵See F. GIUSTINO, M. L. COHEN and S. G. LOUIE, Phys. Rev. B **76**, 165108 (2007) for a methodology review. Results related to ELIASHBERG theory are given by E. R. MARGINE and F. GIUSTINO, Phys. Rev. B **87**, 024505 (2013)

key	default	unit	symbol			ebmb	tc	critical
file	none	–	–	output file		+	+	+
form	F16.12	–	–	number edit descriptor		+	+	+
tell	true	–	–	use standard output?		+	+	+
T	10	K	T	temperature		+	+	+
omegaE	0.02	eV	ω_E	EINSTEIN frequency		+	+	+
cutoff	15	ω_E	ω_N	overall cutoff frequency		+	+	+
cutoffC	ω_N	ω_E	ω_{N_C}	COULOMB cutoff frequency		+	+	+
lambda, lamda	1	1	λ_{ij}	electron-phonon coupling		+	+	+
muStar, mu*	0	1	μ_{ij}^*	rescaled COULOMB potential		+	+	+
muC	0	1	μ_{ij}	unscaled COULOMB parameter		+	+	+
bands	1	1	–	number of bands		+	+	+
dos, DOS	none	–	–	file with density of states		+	+	+
a2f, a2F	none	–	–	file with ELIASHBERG function		+	+	+
n	–	1	n_0	initial occupancy number		+	+	+
mu	0	eV	μ_0	initial chemical potential		+	+	+
conserve	true	–	–	conserve particle number?		+	+	+
chi	true	–	–	consider energy shift?		+	+	+
limit	250000	1	–	maximum number of iterations		+	+	+
epsilon	10^{-13}	a.u.	–	negligible float difference		+	+	+
error	10^{-5}	a.u.	–	bisection error		–	+	+
zero	10^{-10}	eV	–	negligible gap at T_c (threshold)		–	+	–
rate	10^{-1}	1	–	growth rate for bound search		–	+	+
lower	0	eV	–	minimum real-axis frequency		+	–	–
upper	–	eV	–	maximum real-axis frequency		+	–	–
clip	15	ω_E	–	maximum real-axis frequency		+	–	–
eta, 0+	0	eV	–	infinitesimal energy 0^+		+	–	–
resolution	0	1	–	resolution of real-axis solution		+	–	–
measurable	false	–	–	find measurable gap?		+	–	–
unscale	true	–	–	estimate missing muC from mu*?		+	+	+
rescale	true	–	–	use μ_{ij}^* rescaled for cutoff?		+	+	+
imitate	false	–	–	use $Z_i(n)$ biased by cutoff?		–	–	+
normal	false	–	–	enforce normal state?		+	–	–
power	true	–	–	power method for single band?		–	–	+

Table 1: Input parameters.

- The columns ebmb, tc and critical show which keys are used by these programs.
- The rightmost column indicates which parameters may be chosen as variable for critical. The variable is marked with a negative sign; its absolute value is used as initial guess. If no parameter is negative, the critical temperature is searched for.
- lambda, muStar, and muC expect flattened square matrices of equal size the elements of which are separated by commas. It is impossible to vary more than one element at once.
- dos has lines ε/eV $n_1/\text{a.u.}$ $n_2/\text{a.u.}$... with ε ascending but not necessarily equidistant.
- a2F has lines ω/eV $\alpha^2 F_{1,1}$ $\alpha^2 F_{2,1}$... with ω ascending but not necessarily equidistant.

$\langle \text{CHARACTERS key} \rangle : \langle n_1 \times \dots \times n_r \text{ NUMBERS value} \rangle$
 associate key with value
 DIM: $\langle \text{INTEGER } r \rangle \langle r \text{ INTEGERS } n_1 \dots n_r \rangle$
 define shape (column-major)
 INT: take NUMBERS as INTEGERS
 REAL: take NUMBERS as DOUBLES

Table 2: Statements allowed in binary output.
 The data types CHARACTER, INTEGER and DOUBLE
 take 1, 4 and 8 bytes of storage, respectively.

imaginary-axis results			
iomega	MATSUBARA frequency (without i)	ω_n	
Delta	gap	$\Delta_i(n)$	
Z	renormalization	$Z_i(n)$	
chi	energy shift	$\chi_i(n)$	
phiC	constant COULOMB contribution	ϕ_{Ci}	
status	status (steps till convergence or -1)	-	
occupancy results			
n0	initial	} occupancy number	n_0
n	final		n
mu0	initial	} chemical potential	μ_0
mu	final		μ
effective parameters		a2F given	
lambda	electron-phonon coupling	λ_{ij}	
omegaE	EINSTEIN frequency	ω_E	
omegaLog	logarithmic average frequency	ω_{\log}	
omega2nd	second-moment average frequency	$\overline{\omega}_2$	
real-axis results		resolution > 0	
omega	frequency	ω	
Re[Delta]	real	} gap	$\Delta_i(\omega)$
Im[Delta]	imaginary		
Re[Z]	real	} renormalization	$Z_i(\omega)$
Im[Z]	imaginary		
Re[chi]	real	} energy shift	$\chi_i(\omega)$
Im[chi]	imaginary		
measurable results		measurable=true	
Delta0	measurable gap	$\Delta_{0i} = \text{Re}[\Delta_i(\Delta_{0i})]$	
status0	status of measurable gap	-	

Table 3: Keys used in binary output.