ebmb

Solve multiband Eliashberg equations

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. The normal-state equations (Eq. 7) can also be solved on the real axis.

   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 or 6) 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.

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

```
$ make FC=gfortran FFLAGS='-O3 -fopenmp'
$ python3 -m pip install -e .
```

- 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.

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 matrix[1]

$$\boldsymbol{\Sigma}_i(n) = i\omega_n[1 - Z_i(n)]\mathbf{1} + \underbrace{Z_i(n)\,\Delta_i(n)}_{\phi_i(n)}\,\boldsymbol{\sigma}_1 + \chi_i(n)\boldsymbol{\sigma}_3,$$

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 equations[2]

$$Z_i(n) = 1 + \frac{T}{\omega_n}\sum_j\sum_{m=0}^{N-1}\int_{-\infty}^{\infty}\mathrm{d}\varepsilon\,\frac{n_j(\varepsilon)}{n_j(\mu_0)}\,\frac{\omega_m Z_j(m)}{\Theta_j(\varepsilon, m)}\Lambda_{ij}^-(n, m),$$

$$\phi_i(n) = T\sum_j\sum_{m=0}^{N-1}\int_{-\infty}^{\infty}\mathrm{d}\varepsilon\,\frac{n_j(\varepsilon)}{n_j(\mu_0)}\,\frac{\phi_j(m)}{\Theta_j(\varepsilon, m)}[\Lambda_{ij}^+(n, m) - U_{ij}^*(m)],$$

$$\chi_i(n) = \chi_{C_i} - T\sum_j\sum_{m=0}^{N-1}\int_{-\infty}^{\infty}\mathrm{d}\varepsilon\,\frac{n_j(\varepsilon)}{n_j(\mu_0)}\,\frac{\varepsilon - \mu + \chi_j(m)}{\Theta_j(\varepsilon, m)}\Lambda_{ij}^+(n, m),$$

$$\Theta_i(\varepsilon, n) = [\omega_n Z_i(n)]^2 + \phi_i^2(n) + [\varepsilon - \mu + \chi_i(n)]^2,$$

(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

$$\Lambda_{ij}^\pm(n, m) = \lambda_{ij}(n - m) \pm \lambda_{ij}(n + m + 1), \qquad \lambda_{ij}(n) = \int_0^\infty\mathrm{d}\omega\,\frac{2\omega\,\alpha^2 F_{ij}(\omega)}{\omega^2 + \nu_n^2} \underset{\text{Einstein}}{=} \frac{\lambda_{ij}}{1 + \left[\frac{\nu_n}{\omega_E}\right]^2},$$

$$U_{ij}^*(m) = \begin{cases} 2\mu_{ij}^*(\omega_{N_C}) & \text{for } m < N_C, \\ 0 & \text{otherwise,} \end{cases} \qquad \frac{1}{\mu_{ij}^*(\omega_{N_C})} = \frac{1}{\mu_{ij}^*} + \ln\frac{\omega_E}{\omega_{N_C}}$$

(2)

with the ELIASHBERG spectral function $\alpha^2 F_{ij}(\omega)$ and $\mu_{ij}^* = \mu_{ij}^*(\omega_E)$ per definition. Alternatively, if the density of states $n_i(\varepsilon)$ per spin as a function of energy ε is given,

$$\frac{1}{\mu_{ij}^*(\omega_{N_C})} = \frac{1}{\mu_{ij}} + \frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{d}\varepsilon\,\frac{n_j(\varepsilon)}{n_j(\mu_0)}\begin{cases} \frac{1}{\varepsilon - \mu_0}\arctan\frac{\varepsilon - \mu_0}{\omega_{N_C}} & \text{for } \varepsilon \neq \mu_0, \\ \frac{1}{\omega_{N_C}} & \text{otherwise,} \end{cases}$$

(3)

where D is the electronic bandwidth. μ_0 and μ are the chemical potentials for free and interacting particles, whose number n_0, n (including a factor of 2 for the spin) is usually conserved:

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

It is unusual but possible to also consider the COULOMB contribution to the energy shift:

$$\chi_{C_i} = \sum_j\int_{-\infty}^{\infty}\mathrm{d}\varepsilon\,\frac{n_j(\varepsilon)}{n_j(\mu_0)}\left[2T\sum_{m=0}^{N-1}\frac{\varepsilon - \mu + \chi_j(m)}{\Theta_j(\varepsilon, m)} + \frac{1}{\pi}\arctan\frac{\varepsilon - \mu + \chi_{C_j}}{\omega_N}\right]\mu_{ij}.$$

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

[2] G. 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)

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

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 and the second-moment average frequency and use the latter as ω_E in Eqs. 2 and 3 for rescaling μ^*:

$$\omega_{\log} = \exp\left[\frac{2}{\lambda}\int_0^\infty \frac{d\omega}{\omega}\alpha^2 F(\omega)\ln(\omega)\right], \qquad \overline{\omega}_2 = \sqrt{\frac{2}{\lambda}\int_0^\infty d\omega\, \alpha^2 F(\omega)\,\omega}.$$

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

$$Z_i(n) = 1 + \frac{\pi T}{\omega_n}\sum_j \sum_{m=0}^{N-1} \frac{\omega_m}{\sqrt{\omega_m^2 + \Delta_j^2(m)}}\Lambda_{ij}^-(n,m),$$

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

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

$$\phi_i(n) = \sum_j \sum_{m=0}^{N-1} K_{ij}(n,m)\,\phi_j(m),$$

$$K_{ij}(n,m) = T\int_{-\infty}^\infty d\varepsilon\, \frac{n_j(\varepsilon)}{n_j(\mu_0)}\frac{\Lambda_{ij}^+(n,m) - U_{ij}^*(m)}{\Theta_j(\varepsilon,m)}, \tag{5}$$

where $\Theta_j(\varepsilon, m)$ is obtained from Eqs. 1 for $\phi_j(m) = 0$. Similarly, in the constant-DOS case,

$$\Delta_i(n) = \sum_j \sum_{m=0}^{N-1} K_{ij}(n,m)\,\Delta_j(m),$$

$$K_{ij}(n,m) = \frac{1}{2m+1}[\Lambda_{ij}^+(n,m) - \delta_{ij}\delta_{nm}D_i^N(n) - U_{ij}^*(m)],$$

$$D_i^N(n) = \sum_j \sum_{m=0}^{N-1} \Lambda_{ij}^-(n,m) \overset{N=\infty}{=} \sum_j \left[\lambda_{ij} + 2\sum_{m=1}^n \lambda_{ij}(m)\right]. \tag{6}$$

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

The ELIASHBERG equations can also be solved on the real axis,[5] which allows for exact analytic continuation without Padé approximants. They are implemented for the normal state:

$$\Sigma_{11i}(\omega) = \underbrace{\sum_j \int_{-\infty}^\infty d\varepsilon\, \frac{A_j(\varepsilon)}{n_j(\mu_0)}\left[\mu_{ij}\left(\frac{1}{2} - f(\varepsilon)\right)}_{\chi_{C_i}} + \int_0^\infty d\omega'\alpha^2 F_{ij}(\omega')\sum_\pm \pm\frac{f(\varepsilon) + n(\pm\omega')}{\omega - \varepsilon \pm \omega'}\right] \tag{7}$$

with the Fermi function $f(\varepsilon) = 1/(e^{\varepsilon/T} + 1)$ and the Bose function $n(\omega) = 1/(e^{\omega/T} - 1)$. The quasiparticle density of states $A_i(\omega) = -\frac{1}{\pi}\operatorname{Im} G_i(\omega + i\eta)$ follows from the Green function

$$G_i(\omega) = -\int_{-\infty}^\infty d\varepsilon\, n_i(\varepsilon)\frac{\omega Z_i(\omega) + \varepsilon - \mu + \chi_i(\omega)}{\Theta_i(\varepsilon,\omega)} \overset{\phi=0}{=} \int_{-\infty}^\infty d\varepsilon\frac{n_i(\varepsilon)}{\omega - \varepsilon + \mu - \Sigma_{11i}(\omega)}.$$

Note that in the code $\Sigma_{11i}(\omega + i\eta)$ is replaced by $\operatorname{Re}\Sigma_{11i}(\omega + i\eta) + i\operatorname{Im}\Sigma_{11i}(\omega + i0^+)$.

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

[5]D. J. SCALAPINO, J. R. SCHRIEFFER and J. W. WILKINS, Phys. Rev. **148**, 263 (1966). See also L. X. BENEDICT, C. D. SPATARU and S. G. LOUIE, Phys. Rev. B **66**, 085116 (2002)

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key	default	unit	symbol	description	ebmb	tc	critical	variable
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 $\chi_i(n)$?	+	+	+	–
chiC	false	–	–	consider Coulomb part χ_{C_i}?	+	+	+	–
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	ω_N	eV	–	maximum real-axis frequency	+	–	–	–
points	0	1	–	number of real-axis frequencies	+	–	–	–
logscale	1	1/eV	–	scaling of logarithmic sampling	+	–	–	–
eta, 0+	10^{-3}	eV	–	infinitesimal energy 0^+	+	–	–	–
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?	–	–	+	–
divdos	true	–	–	divide by $n_j(\mu_0)$ in Eqs. 1, 3?	+	+	+	–
stable	false	–	–	calculate $A_i(\omega)$ differently?	+	–	–	–
normal	false	–	–	enforce normal state?	+	–	–	–
realgw	false	–	–	do real-axis GW_0 calculation?	+	–	–	–
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/eV^{-1} n_2/eV^{-1} ... 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.
- The relative change in the sample spacing of the real-axis frequencies between $\omega = 0$ and $\omega = x$ is logscale $\cdot |x|$. Thus, logscale $= 0$ corresponds to equidistant sampling.

$\langle\textsc{characters key}\rangle\!:\!\langle n_1 \times \ldots \times n_r \textsc{ numbers value}\rangle$
associate key with value

$\textsf{DIM}\!:\!\langle\textsc{integer } r\rangle\langle r \textsc{ integers } n_1 \ldots n_r\rangle$
define shape (column–major)

$\textsf{INT}\!:$ take $\textsc{numbers}$ as $\textsc{integers}$

$\textsf{REAL}\!:$ take $\textsc{numbers}$ as $\textsc{doubles}$

Table 2: Statements allowed in binary output. The data types $\textsc{character}$, $\textsc{integer}$ and $\textsc{double}$ take 1, 4 and 8 bytes of storage, respectively.

imaginary–axis results		
iomega	$\textsc{Matsubara}$ frequency (without i)	ω_n
Delta	gap	$\Delta_i(n)$
Z	renormalization	$Z_i(n)$
chi	energy shift $(*)$	$\chi_i(n)$
chiC	$\textsc{Coulomb}$ part of energy shift $(*)$	$\chi_{\mathrm{C}i}$
phiC	$\textsc{Coulomb}$ part of order parameter	$\phi_{\mathrm{C}i}$
status	status (steps till convergence or -1)	$-$
occupancy results		$(*)$ DOS given
states	integral of density of states	$\sum_i \int \mathrm{d}\varepsilon\, n_i(\varepsilon)$
inspect	integral of spectral function $(**)$	$\sum_i \int \mathrm{d}\omega\, A_i(\omega)$
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	$\textsc{Einstein}$ frequency	ω_E
omegaLog	logarithmic average frequency	ω_log
omega2nd	second-moment average frequency	$\overline{\omega}_2$
real–axis results		$(**)$ points > 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	
DOS	quasiparticle density of states $(*)$	$A_i(\omega)$
measurable results		measurable=true
Delta0	measurable gap	$\Delta_{0i} = \mathrm{Re}[\Delta_i(\Delta_{0i})]$
status0	status of measurable gap	$-$

Table 3: Keys used in binary output.