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. 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`.

Installation

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

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

Reference

ebmb is stored on *Zenodo:* `https://doi.org/10.5281/zenodo.13341224`.

The theory is described here: `https://scipost.org/theses/132/`.

Licence

Let $\hbar = k_\mathrm{B} = 1$. 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]

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

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]

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

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

$$\begin{aligned}
\Lambda^\pm_{ij}(n,m) &= \lambda_{ij}(n-m) \pm \lambda_{ij}(n+m+1), & \lambda_{ij}(n) &= \int_0^\infty\mathrm{d}\omega\frac{2\omega\,\alpha^2F_{ij}(\omega)}{\omega^2+\nu_n^2} \underset{\text{Einstein}}{\overset{\uparrow}{=}} \frac{\lambda_{ij}}{1+\left[\frac{\nu_n}{\omega_\mathrm{E}}\right]^2},\\
U^*_{ij}(m) &= \begin{cases}2\mu^*_{ij}(\omega_{N_\mathrm{C}}) & \text{for } m < N_\mathrm{C},\\ 0 & \text{otherwise,}\end{cases} & \frac{1}{\mu^*_{ij}(\omega_{N_\mathrm{C}})} &= \frac{1}{\mu^*_{ij}} + \ln\frac{\omega_\mathrm{E}}{\omega_{N_\mathrm{C}}}
\end{aligned}\tag{2}$$

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

$$\frac{1}{\mu^*_{ij}(\omega_{N_\mathrm{C}})} = \frac{1}{\mu_{ij}} + \frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{d}\varepsilon\frac{n_j(\varepsilon)}{n_j(\mu_0)}\begin{cases}\frac{1}{\varepsilon-\mu_0}\arctan\frac{\varepsilon-\mu_0}{\omega_{N_\mathrm{C}}} & \text{for } \varepsilon \neq \mu_0,\\ \frac{1}{\omega_{N_\mathrm{C}}} & \text{otherwise,}\end{cases}\tag{3}$$

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:

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

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

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

[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 $\alpha^2F(\omega)$, 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^*:

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

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

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

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

$$\begin{aligned} \phi_i(n) &= \sum_j\sum_{m=0}^{N-1}K_{ij}(n,m)\,\phi_j(m), \\ K_{ij}(n,m) &= T\int_{-\infty}^\infty \mathrm{d}\varepsilon\frac{n_j(\varepsilon)}{n_j(\mu_0)}\frac{\Lambda_{ij}^+(n,m) - U_{ij}^*(m)}{\Theta_j(\varepsilon,m)}, \end{aligned} \tag{5}$$

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

$$\begin{aligned} \Delta_i(n) &= \sum_j\sum_{m=0}^{N-1}K_{ij}(n,m)\,\Delta_j(m), \\ K_{ij}(n,m) &= \frac{1}{2m+1}[\Lambda_{ij}^+(n,m) - \delta_{ij}\delta_{nm}D_i^N(n) - U_{ij}^*(m)], \\ D_i^N(n) &= \sum_j\sum_{m=0}^{N-1}\Lambda_{ij}^-(n,m) \overset{N=\infty}{=} \sum_j\Big[\lambda_{ij} + 2\sum_{m=1}^{n}\lambda_{ij}(m)\Big]. \end{aligned} \tag{6}$$

$Z_i(n)$ 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:

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

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

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

Note that in the code $\Sigma_{11i}(\omega + \mathrm{i}\eta)$ is replaced by $\operatorname{Re}\Sigma_{11i}(\omega + \mathrm{i}\eta) + \mathrm{i}\operatorname{Im}\Sigma_{11i}(\omega + \mathrm{i}0^+)$.

[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)

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.

  - 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} $\ldots$ with ε increasing.
  - `a2F` has lines ω/eV $\alpha^2F_{1,1}$ $\alpha^2F_{2,1}$ $\ldots$ with ω increasing.
  - The relative change in the sample spacing of the real-axis frequencies between $\omega = 0$ and $\omega = x$ is $\texttt{logscale} \cdot |x|$. Thus, $\texttt{logscale} = 0$ corresponds to equidistant sampling.

- 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.

Acknowledgment

Parts of the program are inspired by the EPW code[6] and work of Malte Rösner.

Contact

Any feedback may be directed to `jan.berges@uni-bremen.de`.

[6]See 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	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 $\chi_{\mathrm{C}i}$?	+	+	+	−
limit	250000	1	–	maximum number of iterations	+	+	+	−
epsilon	10^{-13}	a.u.	–	negligible float difference	+	+	+	−
errorn	10^{-10}	1	–	error of occupancy number	+	+	+	−
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.

⟨CHARACTERS key⟩:⟨$n_1 \times \ldots \times n_r$ NUMBERS value⟩	associate key with value
`DIM:`⟨INTEGER r⟩⟨r INTEGERS $n_1 \ldots n_r$⟩	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 (∗)	$\chi_i(n)$
`chiC`	COULOMB part of energy shift (∗)	$\chi_{\mathrm{C}\,i}$
`phiC`	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 } occupancy number	n
`mu0`	initial } chemical potential	μ_0
`mu`	final } chemical potential	μ
effective parameters		`a2F given`
`lambda`	electron-phonon coupling	λ_{ij}
`omegaE`	EINSTEIN frequency	ω_{E}
`omegaLog`	logarithmic average frequency	$\omega_{\log}$
`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 } gap	
`Re[Z]`	real } renormalization	$Z_i(\omega)$
`Im[Z]`	imaginary } renormalization	
`Re[chi]`	real } energy shift (∗)	$\chi_i(\omega)$
`Im[chi]`	imaginary } energy shift (∗)	
`DOS`	quasiparticle density of states (∗)	$A_i(\omega)$
measurable results		`measurable=true`
`Delta0`	measurable gap	$\Delta_{0\,i} = \mathrm{Re}[\Delta_i(\Delta_{0\,i})]$
`status0`	status of measurable gap	–

Table 3: Keys used in binary output.