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 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]

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

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

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

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

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

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

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:

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

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

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

[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)

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

$$\begin{aligned}
\Delta_i(n) &= \sum_j \sum_{m=0}^{N-1} K_{ij}(n,m)\,\Delta_j(m), \\
K_{ij}(n,m) &= \frac{1}{2m+1}[\Lambda^+_{ij}(n,m) - \delta_{ij}\delta_{nm} D_i^N(n) - U^*_{ij}(m)], \\
D_i^N(n) &= \sum_j \sum_{m=0}^{N-1} \Lambda^-_{ij}(n,m) \overset{N=\infty}{=} \sum_j \Big[\lambda_{ij} + 2\sum_{m=1}^{n} \lambda_{ij}(m)\Big].
\end{aligned} \tag{5}$$

$Z_i(n)$ 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 $\alpha^2F(\omega)$, an effective phonon frequency can be calculated in different ways. We follow Allen and Dynes,[4] who define the logarithmic average frequency

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

and the second-moment average frequency

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

and choose $\overline{\omega}_2$ for ω_{E} in Eqs. 2 and 3 for rescaling μ^*.

Acknowledgment

Parts of the program are inspired by the EPW code[5] and work of Malte Rösner.

Contact

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

[5] 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?	+	+	+	−
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/a.u. n_2/a.u. ... with ε ascending but not necessarily equidistant.
- a2F has lines ω/eV $\alpha^2F_{1,1}$ $\alpha^2F_{2,1}$ ... with ω ascending but not necessarily equidistant.

⟨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	$\chi_i(n)$
`phiC`	constant COULOMB contribution	$\phi_{\mathrm{C}i}$
`status`	status (steps till convergence or -1)	–
occupancy results		
`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		`resolution` > 0
`omega`	frequency	ω
`Re[Delta]`	real gap	$\Delta_i(\omega)$
`Im[Delta]`	imaginary gap	$\Delta_i(\omega)$
`Re[Z]`	real renormalization	$Z_i(\omega)$
`Im[Z]`	imaginary renormalization	$Z_i(\omega)$
`Re[chi]`	real energy shift	$\chi_i(\omega)$
`Im[chi]`	imaginary energy shift	$\chi_i(\omega)$
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.