Solution of the time and energy integration in the derivation of the GME

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Consider

$$\int_0^\infty dt \int_{-\infty}^\infty dE \quad f^{(p)}(E-\mu)\, e^{iqEt}\, e^{i\omega t}\, f^+(E-W_+-\mu) f^-(E-W_--\mu), \tag{1}$$

where

$$f^{(p)}(E) = \frac{1}{e^{p\beta(E)}+1} \tag{2}$$

and $p, q = \pm 1$ respectively. Fermi functions are employed to model an energy band of finite width, $W_+ > 0$ and $W_- < 0$ denoting the band edges. The chemical potential μ shifts both the Fermi level and the band edges and thus appears in all Fermi functions.

For further simplifications one can make a shift in $\tilde{E} = E - \mu$, leading to the following equation:

$$\int_0^\infty dt\, e^{i(\omega+q\mu)t} \int_{-\infty}^\infty dE \quad \frac{1}{e^{p\beta E}+1}\, e^{iqEt}\, \frac{1}{e^{\beta(E-W_+)}+1} \frac{1}{e^{-\beta(E-W_-)}+1}. \tag{3}$$

1 Energy integration

In order to solve the energy integral we use the residue theorem. The poles in the complex plane are:

$$\begin{aligned} e^{p\beta E} = -1 \qquad &\Leftrightarrow \qquad E = i\,\frac{\pi(2n+1)}{\beta} \quad n \in \mathbb{Z}_0\,; \quad \text{residue: } -\frac{p}{\beta}, \\ e^{\alpha\beta(E-W_\alpha)} = -1 \qquad &\Leftrightarrow \qquad E - W_\alpha = i\,\frac{\pi(2n+1)}{\beta} \quad n \in \mathbb{Z}_0; \quad \text{residue: } -\frac{\alpha}{\beta}. \end{aligned} \tag{4}$$

The desired way to close the contour depends only on q, as

$$e^{iq\ i\ \mathrm{Im}(E)t} = e^{-q\mathrm{Im}(E)t}$$

is the part of the integrand which ensures that the contour is vanishing if you send its borders to infinity. For

$$q = \begin{cases} -1 & \text{close contour in lower half plane,} \\ +1 & \text{close contour in the upper half plane,} \end{cases} \tag{5}$$

and thereby follow a path $-M + i0 \to M + i0 \to M + iqN \to M - iqN$ with $M \gg |W_\pm|$ and $N = \frac{2n\pi}{\beta}$, $n \in \mathbb{Z}$, $n \to \infty$. The former ensures that the integrand vanishes on the vertical parts of the path due to the Fermi functions $f^\pm(E - W_\pm)$, the latter lets the contour run in between the poles of the Fermi functions.

Finally we can use the residue theorem to solve the integral. As the choice of the integration way only depends on q and the poles are equally distributed with the same distance $2\pi/\beta$, one can always sum from zero to infinity over the poles $E_0 = iq(2n+1)\pi/\beta$, where q fixes the sign. To consider the cases of integrating clockwise or counterclockwise, the sum over the residues is multiplied by q, yielding a minus sign when integrating over the lower half plane. In total:

$$\begin{aligned}
&\int_{-\infty}^{\infty} dE \quad \frac{1}{e^{p\beta E}+1}\, e^{iqEt}\, \frac{1}{e^{\beta(E-W_+)}+1}\frac{1}{e^{-\beta(E-W_-)}+1} \\
&\quad = 2\pi i\; q \sum_{n=0}^{\infty}\Big(Res_{E_0=iq\frac{(2n+1)\pi}{\beta}}\left[f^{(p)}(E)\right]\; e^{iqE_0t} f^{+}(E_0-W_+) f^{-}(E_0-W_-) \\
&\qquad + \sum_{\alpha=\pm} Res_{E_{0\alpha}=W_\alpha+E_0}\left[f^{\alpha}(E-W_\alpha)\right]\; e^{iqE_{0\alpha}t} f^{(p)}(E_{0\alpha}) f^{-\alpha}(E_{0\alpha}-W_{-\alpha})\Big) \\
&\quad = -\,q\,\frac{2\pi i}{\beta}\;\sum_{n=0}^{\infty}\Big(p\; e^{-\frac{(2n+1)\pi}{\beta}t} + \sum_{\alpha=\pm}\alpha\;\delta_{-\alpha,p}\; e^{iqW_\alpha t}\; e^{-\frac{(2n+1)\pi}{\beta}t}\Big).
\end{aligned}$$

Here we have used the following approximations which hold true for wide bands ($|W_\alpha| \gg k_B T$):

$$\begin{aligned}
f^{\pm}(E_0 - W_\pm) &= \frac{1}{-e^{\mp\beta W_\pm}+1} \approx 1, \\
f^{\mp}(E_{0\pm} - W_\mp) &= \frac{1}{-e^{\mp\beta(W_\pm - W_\mp)}+1} \approx 1, \\
f^{(p)}(E_{0\alpha}) &= \frac{1}{-e^{p\beta W_\alpha}+1} \approx \delta_{p,-\alpha}.
\end{aligned}$$

2 Time integration

Now we are ready to perform the time integral:

$$\begin{aligned}
-pq\;\frac{2\pi i}{\beta}\;\sum_{n=0}^{\infty}\int_0^{\infty} dt\; e^{i(\omega+q\mu)t}\; e^{-\frac{(2n+1)\pi}{\beta}t} &= -pq\;\frac{2\pi i}{\beta}\;\sum_{n=0}^{\infty}\frac{-1}{-(2n+1)\frac{\pi}{\beta}+i(\omega+q\mu)} \\
= pq\;\frac{2\pi i}{\beta}\;\sum_{n=0}^{\infty}\frac{-\beta}{2\pi}\frac{1}{n+\frac{1}{2}-i\frac{(\omega+q\mu)\beta}{2\pi}} &= -i\;pq\;\sum_{n=0}^{\infty}\frac{1}{n+\frac{1}{2}-i\frac{(\omega+q\mu)\beta}{2\pi}},
\end{aligned} \tag{6}$$

and in analogue:

$$-\alpha q\delta_{\alpha,-p}\;\frac{2\pi i}{\beta}\;\sum_{n=0}^{\infty}\int_0^{\infty} dt\; e^{i(\omega+q(\mu+W_\alpha))t}\; e^{-\frac{(2n+1)\pi}{\beta}t} = i\;pq\;\sum_{n=0}^{\infty}\frac{1}{n+\frac{1}{2}-i\frac{(\omega+q(\mu+W_{-p}))\beta}{2\pi}}. \tag{7}$$

As $\frac{(2n+1)\pi}{\beta} > 0$, the integrant goes to zero for $t \to \infty$.
Using the limit representation of the Digammafunction according to
http://functions.wolfram.com/06.14.09.0001.01 :

$$\boxed{\Psi(z) = \lim_{M\to\infty}\Big(\ln M - \sum_{n=0}^{M}\frac{1}{n+z}\Big)} \tag{8}$$

We can write (6)+(7) as:

$$-\,i\;pq\;\left(\lim_{M\to\infty}\ln M - \Psi_0\left(\frac{1}{2}-i\;\frac{(\omega+q\mu)\beta}{2\pi}\right) - \lim_{M\to\infty}\ln M + \Psi_0\left(\frac{1}{2}-i\;\frac{(\omega+q(\mu+W_{-p}))\beta}{2\pi}\right)\right). \tag{9}$$

Now exploiting an identity of the imaginary part of the digammafunction from Abramowitz,

$$\mathrm{Im}\left\{\Psi_0\left(\frac{1}{2}+iy\right)\right\}=\frac{\pi}{2}\ \tanh(\pi y), \tag{10}$$

one can decompose

$$\begin{aligned} iA\ \Psi_0\left(\frac{1}{2}+iy\right) &= iA\ \mathrm{Re}\left\{(\Psi_0\left(\frac{1}{2}+iy\right)\right\}-A\ \mathrm{Im}\left\{\Psi_0\left(\frac{1}{2}+iy\right)\right\} \\ &= iA\ \mathrm{Re}\left\{\Psi_0\left(\frac{1}{2}+iy\right)\right\}-A\ \frac{\pi}{2}\ \tanh(\pi\ y) \end{aligned}$$

and thus

$$\begin{aligned} (7) =& i\ pq\ \left(\mathrm{Re}\left\{\Psi_0\left(\frac{1}{2}-i\ \frac{(\omega+q\mu)\beta}{2\pi}\right)\right\}-\mathrm{Re}\left\{\Psi_0\left(\frac{1}{2}-i\ \frac{(\omega+q(\mu+W_{-p}))\beta}{2\pi}\right)\right\}\right)- \\ &-pq\frac{\pi}{2}\left(\tanh\frac{-\pi(\omega+q\mu)\beta}{2\pi}-\tanh\frac{-\pi(\omega+q(\mu+W_{-p}))\beta}{2\pi}\right). \end{aligned}$$

Rewriting the hyperbolic tangens to a more physical form (i.e., the Fermi function) according to

$$1-\tanh x=1-\frac{e^x-e^{-x}}{e^x+e^{-x}}=2\ \frac{e^{-x}}{e^x+e^{-x}}=\frac{2}{e^{+2x}+1},$$

one obtains:

$$-pq\frac{\pi}{2}\tanh\frac{-(\omega+qy)\beta}{2}=+pq\ \pi\frac{1}{e^{-\beta(\omega+qy)}+1}-pq\frac{\pi}{2}=+pq\ \pi\ \mathrm{f}^{(q)}(-\omega q-y)-pq\ \frac{\pi}{2}.$$

Importantly, for wide bands ($|W_\alpha|\gg k_BT,|\omega|,|\mu|$):

$$\mathrm{f}^{(q)}(-\omega q-\mu-W_{-p})=\frac{1}{e^{q\beta(-\omega q-\mu)}\ e^{-q\beta W_{-p}}+1}\approx\delta_{p,-q}.$$

3 Solution

Finally, the solution can be written as:

$$\begin{aligned} &\int_0^\infty dt\int_{-\infty}^\infty dE\quad f^{(p)}(E-\mu)\ e^{iqEt}\ e^{i\omega t}\ f^+(E-W_+-\mu)f^-(E-W_--\mu) \\ &=i\ pq\ \left[\mathrm{Re}\left\{\Psi_0\left(\frac{1}{2}-i\ \frac{(\omega+q\mu)\beta}{2\pi}\right)\right\}-\mathrm{Re}\left\{\Psi_0\left(\frac{1}{2}-i\ \frac{(\omega+q(\mu+W_{-p}))\beta}{2\pi}\right)\right\}\right] \\ &\quad+pq\ \pi\ \left[\left\{\mathrm{f}^{(+q)}(-\omega q)-\frac{1}{2}\right\}-\left\{\delta_{p,-q}-\frac{1}{2}\right\}\right] \\ &=pq\left[i\ \mathrm{Re}\left\{\Psi_0\left(\frac{1}{2}-i\ \frac{(\omega+q\mu)\beta}{2\pi}\right)\right\}-i\ \mathrm{Re}\left\{\Psi_0\left(\frac{1}{2}-i\ \frac{(\omega+q(\mu+W_{-p}))\beta}{2\pi}\right)\right\}+\pi\mathrm{f}^{(p)}(-\omega q)\right]. \end{aligned}$$