上下接上导线，

在平衡状态（**零偏压**），计算能隙方程，获得有效的吸引势的大小

~~同时验证流是否自动满足守恒~~

1. , int=integral(@(EF) Gless21(EF), -4,0,"ArrayValued",true,'RelTol',1e-4,'AbsTol',1e-13)

|  |  |
| --- | --- |
|  |  |
| -1.99685109222113e-17 - 1.07039557962621i  -2.64781882987105e-17 - 1.07039557962621i  -5.43403351704944e-18 - 1.07039557962621i  5.38616528355725e-17 - 1.07039557962621i  2.67438769564724e-17 - 1.07039557962621i  -1.26802625524235e-17 - 1.07039557962621i  1.61903695877319e-17 - 1.07039557962621i  3.76488707877492e-17 - 1.07039557962621i  2.79513946688966e-17 - 1.07039557962621i  -1.12498053733204e-17 - 1.07039557962621i  -1.61883191222278e-17 - 1.07039557962621i  -1.82334014768805e-17 - 1.07039557962621i  4.44646252555052e-17 - 1.07039557962621i  5.32016228097700e-17 - 1.07039557962621i  2.33803775633334e-17 - 1.07039557962621i  -5.94444796091927e-18 - 1.07039557962621i  2.30287190723870e-17 - 1.07039557962621i  -1.85911555831689e-17 - 1.07039557962621i  -1.93075372869151e-17 - 1.07039557962621i  -2.42723063892099e-17 - 1.07039557962621i  -1.50315101546128e-17 - 1.07039557962621i  5.30639666516556e-18 - 1.07039557962621i  5.97620041828716e-18 - 1.07039557962621i  3.57094455058278e-18 - 1.07039557962621i  -6.31018201125527e-18 - 1.07039557962621i  2.90550429458102e-17 - 1.07039557962621i  -1.23781139833047e-17 - 1.07039557962621i  -2.13855327541156e-17 - 1.07039557962621i  -2.36493369163482e-17 - 1.07039557962621i  8.27130503004664e-18 - 1.07039557962621i | 1.76098970140751 + 3.28517258065817e-17i  1.76098970140751 + 4.35612943415186e-17i  1.76098970140751 + 8.93994448666252e-18i  1.76098970140751 - 8.86119279167348e-17i  1.76098970140751 - 4.39983990895249e-17i  1.76098970140751 + 2.08612705349164e-17i  1.76098970140751 - 2.66360162996314e-17i  1.76098970140751 - 6.19390391634468e-17i  1.76098970140751 - 4.59849789076036e-17i  1.76098970140751 + 1.85079159353162e-17i  1.76098970140751 + 2.66326429218778e-17i  1.76098970140751 + 2.99971644442212e-17i  1.76098970140751 - 7.31521585498627e-17i  1.76098970140751 - 8.75260619993292e-17i  1.76098970140751 - 3.84648487790159e-17i  1.76098970140751 + 9.77966635791528e-18i  1.76098970140751 - 3.78863084778821e-17i  1.76098970140751 + 3.05857331087426e-17i  1.76098970140751 + 3.17643074849693e-17i  1.76098970140751 + 3.99322291631028e-17i  1.76098970140751 + 2.47294879413825e-17i  1.76098970140751 - 8.72995933167328e-18i  1.76098970140751 - 9.83190475602111e-18i  1.76098970140751 - 5.87483421789678e-18i  1.76098970140751 + 1.03813634392136e-17i  1.76098970140751 - 4.78006751666444e-17i  1.76098970140751 + 2.03641827959153e-17i  1.76098970140751 + 3.51829768880973e-17i  1.76098970140751 + 3.89073343981377e-17i  1.76098970140751 - 1.36077570314693e-17i |
|  | Mean value: s1.761 |
|  | Standard value: 1.7480 |

1. , int=integral(@(EF) Gless21(EF), -inf, inf,"ArrayValued", true, 'RelTol',1e-3,'AbsTol',1e-13)

|  |  |
| --- | --- |
|  |  |
| -5.28314521359752e-17 - 1.07814071159653i  9.98267064020732e-17 - 1.07814071159654i  -5.93372904148666e-17 - 1.07814071159653i  1.85510384196600e-17 - 1.07814071159653i  1.79815201478486e-16 - 1.07814071159654i  1.78883359274911e-16 - 1.07814071159654i  -3.16955094668447e-17 - 1.07814071159653i  1.52761774706684e-16 - 1.07814071159653i  1.90935898622039e-16 - 1.07814071159654i  6.47979701113553e-17 - 1.07814071159654i  9.21730467512122e-17 - 1.07814071159654i  -1.09843583181769e-16 - 1.07814071159654i  -1.11401480297734e-16 - 1.07814071159654i  6.58844874836996e-17 - 1.07814071159654i  7.40923131473674e-18 - 1.07814071159653i  2.72431298674712e-16 - 1.07814071159654i  6.16337186697079e-17 - 1.07814071159654i  1.70715383085546e-16 - 1.07814071159653i  -2.75706178288848e-17 - 1.07814071159653i  -3.35163652726710e-17 - 1.07814071159654i  -8.48732757939654e-17 - 1.07814071159654i  5.87608171385115e-17 - 1.07814071159653i  6.32087674626610e-17 - 1.07814071159653i  -1.08960150765896e-16 - 1.07814071159654i  1.78454185477950e-17 - 1.07814071159654i  -1.06478299719664e-16 - 1.07814071159654i  -2.90486272339037e-16 - 1.07814071159654i  -5.23867305047285e-17 - 1.07814071159654i  1.04348450410026e-16 - 1.07814071159654i  1.45147271637832e-17 - 1.07814071159653i | 1.74833912853786 + 8.56727642257578e-17i  1.74833912853786 - 1.61881408427065e-16i  1.74833912853786 + 9.62227893797861e-17i  1.74833912853786 - 3.00828138620909e-17i  1.74833912853786 - 2.91592692186920e-16i  1.74833912853786 - 2.90081594267502e-16i  1.74833912853787 + 5.13982069351302e-17i  1.74833912853786 - 2.47722199145123e-16i  1.74833912853786 - 3.09626284410613e-16i  1.74833912853786 - 1.05077960025968e-16i  1.74833912853786 - 1.49470048295513e-16i  1.74833912853786 + 1.78125018775245e-16i  1.74833912853786 + 1.80651342525738e-16i  1.74833912853786 - 1.06839882950752e-16i  1.74833912853786 - 1.20149892130128e-17i  1.74833912853786 - 4.41781201830385e-16i  1.74833912853786 - 9.99467331383638e-17i  1.74833912853786 - 2.76836205962219e-16i  1.74833912853786 + 4.47091826045815e-17i  1.74833912853786 + 5.43509508752387e-17i  1.74833912853786 + 1.37632562653199e-16i  1.74833912853787 - 9.52879663323240e-17i  1.74833912853786 - 1.02500870464278e-16i  1.74833912853786 + 1.76692423341760e-16i  1.74833912853786 - 2.89385635628617e-17i  1.74833912853786 + 1.72667793487178e-16i  1.74833912853786 + 4.71059585053031e-16i  1.74833912853786 + 8.49515928416769e-17i  1.74833912853786 - 1.69213978186562e-16i  1.74833912853786 - 2.35374336276712e-17i |
|  | Mean value: 1.7483391285 - 4.02766204e-17i |
|  | Standard value: 1.7480 |

1. , int=integral(@(EF) Gless21(EF), -4,0,"ArrayValued",true, 'RelTol',1e-4,'AbsTol',1e-13)

|  |  |
| --- | --- |
|  |  |
| 7.13915868717943e-16 - 1.07887328352756i  -4.91922102987639e-16 - 1.07887328352757i  -7.24571374089669e-16 - 1.07887328352758i  7.93299506674901e-17 - 1.07887328352757i  2.65337062994832e-16 - 1.07887328352755i  8.23267683747605e-16 - 1.07887328352757i  1.44596957496998e-15 - 1.07887328352758i  -1.44203798695113e-15 - 1.07887328352755i  1.75533614025696e-15 - 1.07887328352757i  1.77801072197768e-16 - 1.07887328352757i  3.38436912308126e-16 - 1.07887328352756i  1.01187316376337e-15 - 1.07887328352756i  2.02844408668948e-16 - 1.07887328352757i  1.13235235995809e-15 - 1.07887328352757i  -5.22696159958944e-18 - 1.07887328352756i  -1.14422228334320e-15 - 1.07887328352756i  5.63093097252429e-16 - 1.07887328352757i  3.49521254064753e-16 - 1.07887328352758i  -6.14441056579315e-16 - 1.07887328352757i  -2.42104001916466e-16 - 1.07887328352755i  -1.68557529302419e-15 - 1.07887328352757i  4.54109778923872e-16 - 1.07887328352758i  8.44760123344837e-16 - 1.07887328352755i  6.87142929540423e-16 - 1.07887328352757i  6.28021477399093e-17 - 1.07887328352757i  -7.84571425548873e-16 - 1.07887328352756i  -5.09699973710442e-16 - 1.07887328352756i  5.42550402781736e-17 - 1.07887328352757i  -1.54743769355351e-15 - 1.07887328352756i  -1.28303613862495e-18 - 1.07887328352756i | 1.74715197876686 - 1.15613162523155e-15i  1.74715197876685 + 7.96629862613560e-16i  1.74715197876683 + 1.17338739342896e-15i  1.74715197876684 - 1.28468729739046e-16i  1.74715197876687 - 4.29692885837203e-16i  1.74715197876684 - 1.33321844620287e-15i  1.74715197876683 - 2.34163607785813e-15i  1.74715197876687 + 2.33526917463456e-15i  1.74715197876684 - 2.84263134297229e-15i  1.74715197876684 - 2.87935107727836e-16i  1.74715197876686 - 5.48072447482923e-16i  1.74715197876685 - 1.63865045814258e-15i  1.74715197876685 - 3.28490857451740e-16i  1.74715197876685 - 1.83375721372338e-15i  1.74715197876686 + 8.46466071696716e-18i  1.74715197876686 + 1.85297963812368e-15i  1.74715197876685 - 9.11885792442464e-16i  1.74715197876683 - 5.66022683093617e-16i  1.74715197876684 + 9.95039847801274e-16i  1.74715197876687 + 3.92068737333722e-16i  1.74715197876684 + 2.72965903737892e-15i  1.74715197876683 - 7.35395723425503e-16i  1.74715197876687 - 1.36802379261770e-15i  1.74715197876684 - 1.11277491747391e-15i  1.74715197876684 - 1.01703229072301e-16i  1.74715197876686 + 1.27055284393520e-15i  1.74715197876685 + 8.25419751552186e-16i  1.74715197876685 - 8.78618484926681e-17i  1.74715197876685 + 2.50595586116518e-15i  1.74715197876686 + 2.07777795840721e-18i |
|  | Mean value: 1.747 + 0.0000i |
|  | Standard value: 1.7480 |

**有限偏压的情况**

1. 设定
2. 根据零偏压的情况，有效吸引势
3. 迭代计算
4. 程序计算中，确实可以将积分范围定为正负无穷大。
5. 周期性边界条件下，几乎是均匀的

# 零偏压

需要满足gap方程，所以计算出有效的吸引势

|  |  |  |  |
| --- | --- | --- | --- |
|  | RelTol |  | Time cost |
|  |  | 1.899599583176828 | 2.47 |

Table 1 假设体系在平衡的时候（零偏压），给定上述参数的情况下，保证 ，得到有效吸引势

# 有限偏压

1. 迭代计算能隙

* 首先，我先假设中心区的化学势不变。

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| 迭代次数 |  |  | | RelErr= | AbsErr |
| 1 | 0.6 | 0.299783682393242 + 0.000873165565592i | | (-7.21e-04, +Inf) | (-2.16e-04, +8.73e-04) |
| 2 | 0.6 | 0.299644065756453 + 0.000001636062293i | | (-4.66e-04, -9.98e-01) | (-1.40e-04, -8.72e-04) |
| 3 | 0.6 | 0.299550452185564 + 0.000873560141043i | | (-3.12e-04, +5.33e+02) | (-9.36e-05, +8.72e-04) |
| 4 | 0.6 | 0.299491189693825 + 0.000002339935268i | | (-1.98e-04, -9.97e-01) | (-5.93e-05, -8.71e-04) |
| 5 | 0.6 |  | |  |  |
| 接下来，改变化学势到，继续迭代 | | |  | | |
| 6 | 0.65 | 0.293412888720979 - 0.000085172027486i | | [-0.0013,-1.1048] |  |
| 7 | 0.65 | 0.295731747888923 + 0.000008865028269i | | [0.0079,-1.1041] |  |
| 8 | 0.65 | 0.297009105762161 - 0.000000928447838i | | [0.0043,-1.1047] |  |
| 9 | 0.65 | 0.297888264402383 + 0.000000097530335i | | (+2.96e-03, -1.11e+00) | (+8.79e-04, +1.03e-06) |

1. 检验电流是否自动守恒