

# Numeric Computation of BCS Superfluid Stiffness

Ethan Huecker

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**Preface:** This was my first research project as a graduate student, and was devised to help myself gain familiarity with field-theoretic approaches to BCS superconductivity and numerical approaches to continuum systems.

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Our goal is the numeric computation of the superfluid stiffness of a BCS superconductor. In doing so, I will work within a  $2d$  tight-binding model with dispersion

$$\varepsilon_{\mathbf{k}} = -\frac{1}{m} (\cos(k_x) + \cos(k_y)), \quad (1)$$

where  $2t = 1/m$  was chosen so that for small momenta the dispersion is the usual kinetic term of free electrons.<sup>1</sup> This requires a near circular Fermi surface generated through the condition that

$$\frac{2\pi}{L} \ll k_F \ll 2\pi, \quad (2)$$

avoiding edge effects with the BZ and grid size. For this choice, the lattice model stiffness will simplify to that of a continuum model which can be directly compared to known results, such as that of Altland and Simons' text [1].

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Note Altland and Simons' calculation for the stiffness,

$$\begin{aligned} \frac{n_s}{2m} &= \frac{n}{2m} - \frac{\beta}{4m^2 L^2} \sum_{\mathbf{k}} |\mathbf{k}|^2 n_F(\lambda_{\mathbf{k}}) (1 - n_F(\lambda_{\mathbf{k}})) = \frac{n}{2m} + \frac{1}{4m^2} \int_{-\infty}^{\infty} d\xi \nu(\xi) |\mathbf{k}|^2 n'_F(\lambda_{\mathbf{k}}) \\ &\approx \frac{n}{2m} + \frac{\mu\nu}{2m} \int_{-\infty}^{\infty} d\xi n'_F(\lambda_{\mathbf{k}}) \\ \iff \frac{n_s}{n} &\approx 1 + \int_{-\infty}^{\infty} d\xi n'_F(\lambda_{\mathbf{k}}), \end{aligned} \quad (3)$$

where  $\lambda_{\mathbf{k}} \equiv \sqrt{\xi^2 + \Delta^2}$ , for  $\xi = \varepsilon_{\mathbf{k}} - \mu$ , and  $n = \mu\nu$  in  $2d$ , they assume the integrand is peaked at the Fermi surface and take  $|\mathbf{k}|^2 \sim k_F^2$  with flat density of states  $\nu$ . A comparison of the result (3) with the numerical evaluation of the lattice model is valid if the numerical evaluation is performed under these approximations. As justification, it must be that

$$\varepsilon_F \gg T, \Delta \quad (4)$$

where for the lattice model,  $\varepsilon_F = |\mu + 2/m|$  is the difference between the Fermi level and the bottom of the band. This ensures that the integrand is peaked on some energy scale much smaller than the Fermi energy, as the function  $n'_F(\lambda_{\mathbf{k}})$  has a peak of width  $\sim T$ .

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<sup>1</sup>Through a suitable choice of the chemical potential, the constant  $-2/m$  is absorbed.

I will compute the stiffness through gauge coupling, which for a lattice model is performed via a Peierl's substitution. For the 1d case,

$$\begin{aligned}
H_t &= -t \sum_{j,\sigma} \left( c_{j,\sigma}^\dagger c_{j+1,\sigma} + \text{h.c.} \right) \rightarrow -t \sum_{j,\sigma} \left( c_{j,\sigma}^\dagger c_{j+1,\sigma} e^{-iqA} + \text{h.c.} \right) \\
&= -t \sum_{k,k',\sigma} \sum_j \left( c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',\sigma} e^{-ikj} e^{ik(j+1)} e^{-iqA} + \text{h.c.} \right) \\
&= -t \sum_{k,\sigma} \left( c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma} e^{i(k-qA)} + \text{h.c.} \right) \\
&= \sum_{\mathbf{k},\sigma} (-2t \cos(k - qA)) c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma},
\end{aligned} \tag{5}$$

where I took the gauge field to be site-independent. The generalization to 2d is then simply

$$\varepsilon_{\mathbf{k}}(\mathbf{A}) = -\frac{1}{m} (\cos(k_x + A_x) + \cos(k_y + A_y)). \tag{6}$$

To determine the interaction vertices, I will implement a trig identity and expand for small  $A$ ,

$$\begin{aligned}
\varepsilon_{\mathbf{k}}(\mathbf{A}) &= -\frac{1}{m} (\cos(k_x) \cos(A_x) - \sin(k_x) \sin(A_x) + \cos(k_y) \cos(A_y) - \sin(k_y) \sin(A_y)) \\
&= \varepsilon_{\mathbf{k}}(0) + \frac{\sin(k_x)}{m} A_x + \frac{\sin(k_y)}{m} A_y + \frac{\cos(k_x)}{2m} A_x^2 + \frac{\cos(k_y)}{2m} A_y^2,
\end{aligned} \tag{7}$$

and so I find two 3-point vertices and two 4-point vertices. For Nambu Green's functions, the 4-point vertex must come with an additional  $\tau_3$  as result of the hole dispersion.

The diamagnetic and paramagnetic contributions to the superfluid density then take the form

$$\begin{aligned}
\frac{n_s}{2m} &= \text{diagram 1} + \text{diagram 2} \\
&= \frac{T}{L^2} \sum_{i\omega_n} \sum_{k_x, k_y} \text{tr} \left[ \mathcal{G}_{\mathbf{k}} \tau_3 \frac{\cos(k_x)}{2m} \right] + \frac{T}{2L^2} \sum_{i\omega_n} \sum_{k_x, k_y} \text{tr} \left[ \mathcal{G}_{\mathbf{k}} \tau_0 \frac{\sin(k_x)}{m} \mathcal{G}_{\mathbf{k}} \tau_0 \frac{\sin(k_x)}{m} \right] \\
&= \frac{T}{2mL^2} \sum_{i\omega_n} \sum_{k_x, k_y} \cos(k_x) \text{tr} [\mathcal{G}_{\mathbf{k}} \tau_3] + \frac{T}{2m^2 L^2} \sum_{i\omega_n} \sum_{k_x, k_y} \sin^2(k_x) \text{tr} [\mathcal{G}_{\mathbf{k}} \mathcal{G}_{\mathbf{k}}],
\end{aligned} \tag{8}$$

where

$$\mathcal{G}_{\mathbf{k}} = \begin{pmatrix} i\omega_n - \xi_{\mathbf{k}} & -\Delta \\ -\Delta & i\omega_n + \xi_{\mathbf{k}} \end{pmatrix}^{-1} = \frac{1}{(i\omega_n)^2 - \xi_{\mathbf{k}}^2 - |\Delta|^2} \begin{pmatrix} i\omega_n + \xi_{\mathbf{k}} & \Delta \\ \Delta & i\omega_n - \xi_{\mathbf{k}} \end{pmatrix} \tag{9}$$

is the Nambu Green's function for  $\xi_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu$ , and I am defining lowercase  $\text{tr}[\dots]$  to run only over Nambu space. It is implicit that the momentum sums run over the 1BZ from  $[-\pi, \pi)$ .

As exercise I will fully simplify the diamagnetic term (8),

$$\begin{aligned}
\text{Tr}[\mathcal{G}_{\mathbf{k}}\tau_3 \frac{\cos(k_x)}{2m}] &= \frac{T}{2mL^2} \sum_{\mathbf{k}} \sum_{i\omega_n} \cos(k_x) \left[ \frac{i\omega_n + \xi_{\mathbf{k}}}{(i\omega_n)^2 - \xi_{\mathbf{k}}^2 - |\Delta|^2} e^{i\omega_n 0^+} - \frac{i\omega_n - \xi_{\mathbf{k}}}{(i\omega_n)^2 - \xi_{\mathbf{k}}^2 - |\Delta|^2} e^{-i\omega_n 0^+} \right] \\
&= \frac{1}{2m\beta L^2} \sum_{\mathbf{k}} \cos(k_x) \oint \frac{dz}{2\pi i} \left[ \frac{(z + \xi_{\mathbf{k}})e^{z0^+}}{(z - \lambda_{\mathbf{k}})(z + \lambda_{\mathbf{k}})} \left( -\frac{\beta}{e^{\beta z} + 1} \right) - \frac{(z - \xi_{\mathbf{k}})e^{-z0^+}}{(z - \lambda_{\mathbf{k}})(z + \lambda_{\mathbf{k}})} \left( \frac{\beta}{1 + e^{-\beta z}} \right) \right] \\
&= \frac{1}{2mL^2} \sum_{\mathbf{k}} \cos(k_x) \sum_{z=\pm\lambda_{\mathbf{k}}} \text{Res} \left[ \frac{(z + \xi_{\mathbf{k}})}{(z - \lambda_{\mathbf{k}})(z + \lambda_{\mathbf{k}})} \left( \frac{1}{e^{\beta z} + 1} \right) + \frac{(z - \xi_{\mathbf{k}})}{(z - \lambda_{\mathbf{k}})(z + \lambda_{\mathbf{k}})} \left( \frac{1}{1 + e^{-\beta z}} \right) \right] \quad (10) \\
&= \frac{1}{2mL^2} \sum_{\mathbf{k}} \cos(k_x) \left[ \frac{(\lambda_{\mathbf{k}} + \xi_{\mathbf{k}})n_F(\lambda_{\mathbf{k}}) + (\lambda_{\mathbf{k}} - \xi_{\mathbf{k}})n_F(-\lambda_{\mathbf{k}})}{\lambda_{\mathbf{k}}} \right] \\
&= \frac{1}{2mL^2} \sum_{\mathbf{k}} \cos(k_x) \left[ \frac{\sqrt{\xi_{\mathbf{k}}^2 + \Delta^2} - \xi_{\mathbf{k}} + 2\xi_{\mathbf{k}}n_F(\sqrt{\xi_{\mathbf{k}}^2 + \Delta^2})}{\sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}} \right],
\end{aligned}$$

where as above I defined  $\lambda_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta^2}$ . Does (10) agree with the particle density for a normal metal ( $\Delta = 0$ ), in the non-lattice model? In that case,  $\lambda_{\mathbf{k}} = \xi_{\mathbf{k}}$  and I make the continuum replacement  $\cos(k_x) \rightarrow 1$ , such that

$$\text{Tr}[\mathcal{G}_{\mathbf{k}}\tau_3] = \frac{1}{L^2} \sum_{\mathbf{k}} 2n_F(\xi_{\mathbf{k}}) = n_0, \quad (11)$$

which is indeed the (spinful) particle density  $n_0$  in the absence of superconductivity.

## Numerics

It is at this point that the diagrams (8) can be evaluated using software like Mathematica. I computed the trace over Nambu space first, then performed the Matsubara sum directly, substituting  $i\omega_n \rightarrow i\pi T(2n + 1)$  for  $n \in \mathbb{Z}$ . Consistent results were found with a frequency cutoff of  $n_{\text{max}} \sim 10,000$ . Care was taken in order to ensure the convergence of the sum; the paramagnetic term (8) contains  $\mathcal{G}_{\mathbf{k}}^2$  and hence converges over the whole complex plane, but the diamagnetic term does not, as illustrated in (10). To alleviate this, I manually distributed Matsubara weighting functions to each term.

As a way of viewing the behavior of  $n_s/2m$ , I instead divided it by the diamagnetic term to get  $n_s/n$ , which should be 1 at low temperatures and vanish as  $T$  becomes large. This is shown below in Fig.[1]. I also compare the numerical evaluation of the lattice model Fig.[1] to that of the continuum result (3) in Fig.[2]. The deviation between the two is not significant, growing as  $T$  increases; this is an artifact of the lattice model approximation.

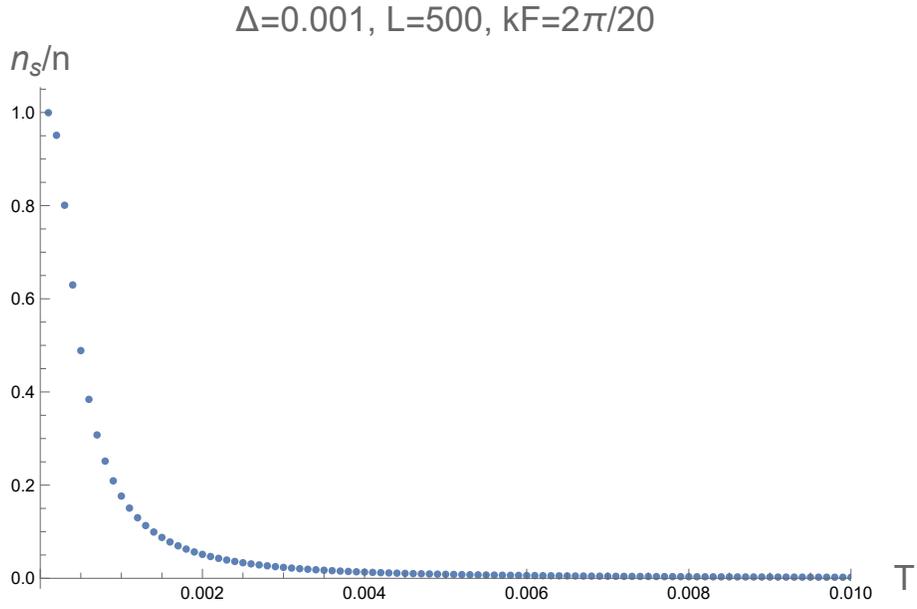


Figure 1: Numerical evaluation (8) for  $n_s/n$ , with expected behavior for  $T \in [0, 0.01]$ . Note the onset of condensation indeed occurs around  $T \sim \Delta$ .

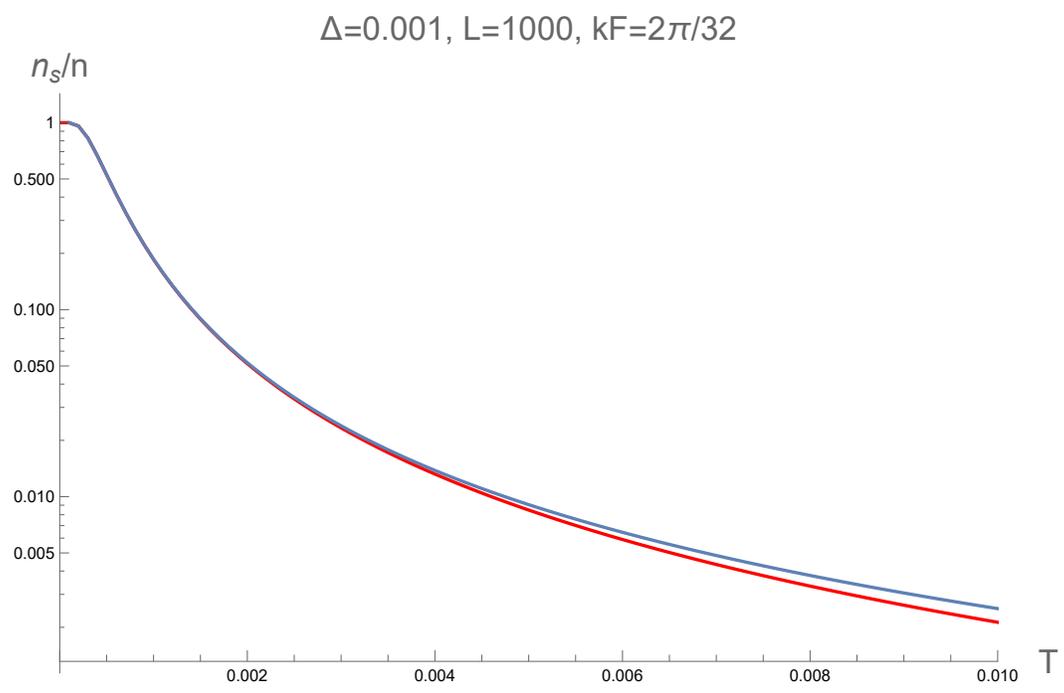


Figure 2: Log plot of lattice model  $n_s/n$  (blue) vs. the continuum result (3) (red). The agreement improves as  $L$  increases and  $k_F$  decreases.

## References

[1] Alexander Altland and Ben D. Simons. *Condensed Matter Field Theory*. Cambridge University Press, 3 edition, 2023.