

Quasiparticle Density and Dynamics in Superconductors

Soren Ormseth

June 2025

1 Quasiparticle Density

Let N_{qp} be the total number of quasiparticles in a superconductor. The spectral density of these quasiparticles, denoted $N(E, \mathbf{r})$, represents the number of quasiparticles per unit volume per unit energy at position \mathbf{r} and energy E . The total number is found by integrating this density over the volume and all allowed quasiparticle energies:

$$N_{\text{qp}} = \int_V \int_{\text{allowed } E} N(E, \mathbf{r}) dE dV. \quad (1)$$

In a superconductor with an energy gap $\Delta(\mathbf{r})$, there are no quasiparticle states for $E < \Delta(\mathbf{r})$, so the integral is taken from the gap edge to infinity.

1.1 Momentum-Space Representation

To understand the origin of the quasiparticle states, we first consider the ground state of the superconductor in the BCS framework. This state is a coherent superposition of Cooper-paired electron states, represented by the wavefunction:

$$|\Psi_0\rangle = \prod_{\mathbf{k}} \left(u_{\mathbf{k}} + v_{\mathbf{k}} c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow}^\dagger \right) |0\rangle, \quad (2)$$

where $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are the BCS coherence factors and c^\dagger are electron creation operators. Quasiparticles are the elementary excitations above this ground state. We can express their energy in terms of the kinetic energy of the normal-state electrons relative to the Fermi level, $\epsilon = p^2/2m - \epsilon_F$. The quasiparticle energy is then given by the Bogoliubov dispersion relation:

$$E(\epsilon) = \sqrt{\epsilon^2 + \Delta^2}. \quad (3)$$

In this representation, the total number of quasiparticles is found by integrating over all electron and hole states. For a spatially uniform gap Δ , this is:

$$N_{\text{qp}} = \int_V \int_{-\epsilon_F}^{+\infty} 2N(0) f(E(\epsilon)) d\epsilon \approx \int_V \int_{-\infty}^{+\infty} 2N(0) f(E(\epsilon)) d\epsilon. \quad (4)$$

Here $N(0)$ is the *single*-spin density of states at the Fermi level (approximated as constant), and hence the factor of 2 appears. The function $f(E)$ is the occupation probability of a state with energy E . In thermal equilibrium, it is the Fermi-Dirac distribution:

$$f(E, T) = \frac{1}{e^{E/(k_B T)} + 1}. \quad (5)$$

The error introduced by changing the lower limit of integration to $-\infty$ is negligible because $f(E(-\epsilon_F))$ is effectively zero for typical energy scales, which is the case when $f(E)$ is a Fermi-Dirac distribution at any relevant temperature.

1.1.1 Transformation to Energy Space

We can transform the momentum-space integral (Eq. 4) back into the energy-space representation of Eq. (1) to find an explicit expression for the spectral density $N(E, \mathbf{r})$. First, we note the differential relation from $E = \sqrt{\epsilon^2 + \Delta^2}$:

$$d\epsilon = \frac{E}{\sqrt{E^2 - \Delta^2}} dE. \quad (6)$$

The mapping $E(\epsilon)$ is two-to-one: both $\epsilon > 0$ (electron-like) and $\epsilon < 0$ (hole-like) map to the same quasiparticle energy E . We can therefore split the integral over ϵ and use its symmetry, $E(\epsilon) = E(-\epsilon)$:

$$\begin{aligned} N_{\text{qp}} &= \int_V \left(\int_{-\infty}^0 2N(0)f(E(\epsilon)) d\epsilon + \int_0^{+\infty} 2N(0)f(E(\epsilon)) d\epsilon \right) dV \\ &= \int_V \int_0^{+\infty} 4N(0)f(E(\epsilon)) d\epsilon dV. \end{aligned} \quad (7)$$

Changing variables from ϵ to E (where $\epsilon \in [0, \infty)$ maps to $E \in [\Delta, \infty)$) yields:

$$N_{\text{qp}} = \int_V \int_{\Delta}^{\infty} 4N(0)f(E) \frac{E}{\sqrt{E^2 - \Delta^2}} dE dV. \quad (8)$$

Comparing this result with Eq. (1) provides the explicit form of the spectral density. Generalizing to the case where properties may vary spatially, we get:

$$N(E, \mathbf{r}) = 4N(0, \mathbf{r}) \frac{E}{\sqrt{E^2 - \Delta(\mathbf{r})^2}} f(E, \mathbf{r}), \quad \text{for } E \geq \Delta(\mathbf{r}). \quad (9)$$

Even if the underlying material is chemically homogeneous, the gap $\Delta(\mathbf{r})$ may vary because of, for example, local variations in the thickness of a superconducting film. In these cases, the normal-state density of states $N(0)$ can still be treated as spatially uniform and factored out of the volume integral.

Doing so allows us to define a set of related quantities which are convenient for analysis and simulation. First, we define the **normalized BCS density of states**:

$$\rho(E, \mathbf{r}) = \frac{E}{\sqrt{E^2 - \Delta(\mathbf{r})^2}}. \quad (10)$$

This expression for $\rho(E, \mathbf{r})$ has a singularity at the gap edge, $E = \Delta$. In many practical situations, particularly when comparing with experimental data, it is useful to include a phenomenological lifetime broadening effect. This is accomplished using the **Dynes density of states**, which introduces a broadening parameter Γ :

$$\rho(E, \mathbf{r}, \Gamma) = \text{Re} \left\{ \frac{E - i\Gamma}{\sqrt{(E - i\Gamma)^2 - \Delta(\mathbf{r})^2}} \right\}. \quad (11)$$

The parameter Γ accounts for processes that give quasiparticle states a finite lifetime, smearing the singularity at the gap edge.

The product of this with the occupation probability gives the **normalized quasiparticle spectral density**, a useful dimensionless quantity:

$$n(E, \mathbf{r}) = \rho(E, \mathbf{r}) f(E, \mathbf{r}). \quad (12)$$

Integrating this distribution over all allowed energies gives the **local quasiparticle density parameter**:

$$x_{\text{qp}}(\mathbf{r}) = \int_{\Delta(\mathbf{r})}^{\infty} n(E, \mathbf{r}) dE. \quad (13)$$

This quantity, which has units of energy, is sometimes referred to as a dimensionless density in the literature, a convention that arises if it is implicitly normalized by a characteristic energy like Δ_0 or $k_B T_c$. The total number of quasiparticles is then simply:

$$N_{\text{qp}} = 4N(0) \int_V x_{\text{qp}}(\mathbf{r}) dV. \quad (14)$$

For non-equilibrium problems, the occupation probability $f(E, \mathbf{r})$ may be an arbitrary distribution. In such cases, some of the initial assumptions must be revisited. Specifically, the approximation of extending the integration limit in Eq. (4) to $-\infty$ and the assumption of a constant normal-state density of states, $N(\epsilon) \approx N(0)$, both rely on the relevant physics being confined to a narrow energy window around the Fermi level. If a highly non-equilibrium distribution significantly populates states with large $|\epsilon|$, these approximations could introduce significant errors. However, for many practical non-equilibrium scenarios where the quasiparticle distribution is still primarily concentrated near the gap edge, these standard simplifications remain highly effective.

2 Quasiparticle Dynamics: The Master Equation

To model the time evolution of the quasiparticle population, we formulate a master equation for the quasiparticle density. For simplicity, we assume spatial homogeneity and work with the dimensionless spectral density $n(E, t)$. The dominant kinetic processes that we will consider are: quasiparticle-phonon scattering, quasiparticle-quasiparticle recombination, thermal (phonon-mediated)

quasiparticle generation, and external sources. We ignore quasiparticle-lattice impurity scattering and quasiparticle-quasiparticle scattering. The master equation can be written conceptually as:

$$\frac{\partial n(E, t)}{\partial t} = \text{Generation} + \text{Scattering In} - \text{Scattering Out} - \text{Recombination}. \quad (15)$$

We examine each process:

- **External Generation** represents quasiparticle creation from external sources such as stray infrared photons, cosmic rays, other high-energy particle impacts, direct quasiparticle injection, or non-equilibrium phonon-mediated generation. This is denoted by a dimensionless rate $g_{\text{ext}}(E)$.
- **Thermal Generation** occurs when thermal phonons with energy $\geq 2\Delta$ break Cooper pairs. We derive this term later via detailed balance.
- **Scattering** redistributes quasiparticles in energy through phonon exchange. The rates depend on the scattering kernel $K^s(E, E')$ from Martinis et al. [1] and Lenander et al. [2]:

$$K^s(E, E') = \frac{1}{\tau_0} \frac{(E - E')^2}{(k_B T_c)^3} \left(1 - \frac{\Delta^2}{EE'}\right) N_p(E - E'), \quad (16)$$

where τ_0 is a material-specific electron-phonon interaction time, T_c is the critical temperature, $(1 - \Delta^2/EE')$ is the BCS coherence factor, and $N_p(E_{\text{e-ph}})$ is the effective phonon occupation factor.¹

- **Recombination** removes quasiparticles when two of them combine to form a Cooper pair. The rate depends on the recombination kernel $K^r(E, E')$, also from Martinis et al. [1] and Lenander et al. [2]:

$$K^r(E, E') = \frac{1}{\tau_0} \frac{(E + E')^2}{(k_B T_c)^3} \left(1 + \frac{\Delta^2}{EE'}\right) N_p(E + E'). \quad (17)$$

The full master equation for the dimensionless quasiparticle density $n(E, t)$ is:

$$\begin{aligned} \frac{\partial n(E, t)}{\partial t} = & g_{\text{ext}}(E) + G_{\text{therm}}(E) \\ & + \int_{\Delta}^{\infty} n(E') K^s(E', E) \rho(E) \left[1 - \frac{n(E)}{\rho(E)}\right] dE' \\ & - n(E) \int_{\Delta}^{\infty} K^s(E, E') \rho(E') \left[1 - \frac{n(E')}{\rho(E')}\right] dE' \\ & - 2n(E) \int_{\Delta}^{\infty} K^r(E, E') n(E') dE'. \end{aligned} \quad (18)$$

¹The phonon occupation factor $N_p(E_{\text{e-ph}})$ is a compact notation that handles both phonon emission and absorption. For a thermal phonon bath at temperature T_p , it is given by $N_p(E_{\text{e-ph}}) = 1/|\exp(-E_{\text{e-ph}}/k_B T_p) - 1|$. When a quasiparticle emits a phonon ($E_{\text{e-ph}} > 0$), this term evaluates to $1 + n_{BE}(E_{\text{e-ph}})$. When it absorbs a phonon ($E_{\text{e-ph}} < 0$), it evaluates to $n_{BE}(|E_{\text{e-ph}}|)$.

The Pauli blocking factor is written as $[1 - f(E)] = [1 - n(E)/\rho(E)]$. The factor of 2 in the recombination term arises because the loss of a quasiparticle at energy E is due to its recombination with a quasiparticle at any other energy E' , and this process is symmetric [3]. For brevity, the entire right-hand side of Eq. (18), representing all local generation and kinetic processes, is often collected into a single term called the **collision integral**, $\mathcal{I}_{\text{coll}}[n]$.

2.1 Determination of Thermal Generation Rate

We derive the thermal generation rate $G_{\text{therm}}(E)$ by invoking the principle of detailed balance. We assume the system is in thermal equilibrium at temperature T . The quasiparticle density is given by the Fermi-Dirac distribution, $n_{\text{eq}}(E, T) = \rho(E)f_{\text{eq}}(E, T)$, where $f_{\text{eq}}(E, T) = (e^{E/k_B T} + 1)^{-1}$, and the phonons are described by a Bose-Einstein distribution.

At equilibrium, the net rate of change for any process must be zero. For scattering, this means the scattering-in and scattering-out rates must be equal. This equality is guaranteed by a fundamental property of the scattering kernel:

$$K^s(E, E') = K^s(E', E)e^{(E-E')/k_B T}. \quad (19)$$

2.1.1 Derivation of the Kernel Balance Property

The kernel property in Eq. (19) arises from the Bose-Einstein statistics of the mediating phonons, encapsulated in the term $N_p(E_{\text{e-ph}})$. Letting $x = (E - E')/k_B T$, the property is equivalent to proving the identity $N_p(-x) = N_p(x)e^{-x}$, or:

$$\frac{1}{|\exp(x) - 1|} = \frac{e^{-x}}{|\exp(-x) - 1|}. \quad (20)$$

We prove this by starting with the right-hand side:

$$\begin{aligned} \frac{e^{-x}}{|\exp(-x) - 1|} &= \frac{e^{-x}}{|e^{-x}(1 - e^x)|} = \frac{e^{-x}}{|e^{-x}| \cdot |1 - e^x|} \\ &= \frac{e^{-x}}{e^{-x}|1 - e^x|} \quad (\text{since } e^{-x} > 0) \\ &= \frac{1}{|1 - e^x|} = \frac{1}{|e^x - 1|}. \end{aligned}$$

This confirms the detailed balance relation for the scattering kernel.

2.1.2 Proof of Scattering Rate Balance at Equilibrium

We now explicitly show that the kernel property in Eq. (19) ensures that the total scattering-in rate equals the total scattering-out rate at thermal equilibrium.

The scattering-in and scattering-out rates to energy E are given by:

$$\text{Rate In}(E) = \int_{\Delta}^{\infty} n_{\text{eq}}(E') K^s(E', E) \rho(E) [1 - f_{\text{eq}}(E)] dE' \quad (21)$$

$$\text{Rate Out}(E) = n_{\text{eq}}(E) \int_{\Delta}^{\infty} K^s(E, E') \rho(E') [1 - f_{\text{eq}}(E')] dE'. \quad (22)$$

To prove these are equal, we transform the “Rate In” expression using equilibrium relationships. First, substitute the kernel property from Eq. (19) and the definition $n_{\text{eq}}(E') = \rho(E') f_{\text{eq}}(E')$:

$$\text{Rate In}(E) = \int_{\Delta}^{\infty} \rho(E') f_{\text{eq}}(E') \left(K^s(E, E') e^{(E'-E)/k_B T} \right) \rho(E) [1 - f_{\text{eq}}(E)] dE'. \quad (23)$$

A key identity for fermions in thermal equilibrium is $f_{\text{eq}}(E') [1 - f_{\text{eq}}(E)] e^{(E'-E)/k_B T} = f_{\text{eq}}(E) [1 - f_{\text{eq}}(E')]$. Substituting this gives:

$$\text{Rate In}(E) = \int_{\Delta}^{\infty} K^s(E, E') \rho(E') \rho(E) (f_{\text{eq}}(E) [1 - f_{\text{eq}}(E')]) dE'. \quad (24)$$

Rearranging and recognizing that $\rho(E) f_{\text{eq}}(E) = n_{\text{eq}}(E)$ yields the desired result:

$$\text{Rate In}(E) = n_{\text{eq}}(E) \int_{\Delta}^{\infty} K^s(E, E') \rho(E') [1 - f_{\text{eq}}(E')] dE' = \text{Rate Out}(E). \quad (25)$$

Thus, the net scattering contribution at thermal equilibrium is zero.

2.1.3 Thermal Generation Rate

With the net scattering rate confirmed to be zero, the master equation at equilibrium ($\partial n / \partial t = 0$) with no external sources ($g_{\text{ext}} = 0$) simplifies to a balance between thermal generation and recombination:

$$0 = G_{\text{therm}}(E) - \text{Recombination}_{\text{eq}} = G_{\text{therm}}(E) - 2n_{\text{eq}}(E) \int_{\Delta}^{\infty} K^r(E, E') n_{\text{eq}}(E') dE'. \quad (26)$$

Therefore, the thermal generation rate required to maintain equilibrium is:

$$G_{\text{therm}}(E) = 2n_{\text{eq}}(E) \int_{\Delta}^{\infty} K^r(E, E') n_{\text{eq}}(E') dE'. \quad (27)$$

Substituting this back into Eq. (18) gives the final master equation.

3 Spatially-Resolved Dynamics: The Reaction-Diffusion Equation

To model systems with spatial inhomogeneity, we must include a transport term. Assuming quasiparticle motion is diffusive, the full dynamics of the spectral

density $n(E, \mathbf{r}, t)$ are described by a reaction-diffusion equation:

$$\frac{\partial n(E, \mathbf{r}, t)}{\partial t} = \nabla \cdot [D(E, n, \mathbf{r}) \nabla n(E, \mathbf{r}, t)] + \mathcal{I}_{\text{coll}}[n(E, \mathbf{r}, t)], \quad (28)$$

where $D(E, n, \mathbf{r})$ is the diffusion coefficient. Its dependence on position \mathbf{r} arises primarily from the local energy gap $\Delta(\mathbf{r})$, and Δ may also in turn depend on the quasiparticle density n . The term $\mathcal{I}_{\text{coll}}$ is the collision integral, representing all local generation and kinetic terms as defined on the right-hand side of Eq. (18).

In one dimension, the diffusion term expands as:

$$\frac{\partial}{\partial x} \left[D \frac{\partial n}{\partial x} \right] = \frac{\partial D}{\partial x} \frac{\partial n}{\partial x} + D \frac{\partial^2 n}{\partial x^2}. \quad (29)$$

Because the diffusion coefficient D can depend on the density n , the chain rule must be applied carefully: $\frac{\partial D}{\partial x} = \frac{\partial D}{\partial n} \frac{\partial n}{\partial x} + \dots$. This introduces a term proportional to $(\partial n / \partial x)^2$, making the full reaction-diffusion equation non-linear.

3.1 Energy-Dependent Diffusion Coefficient

The energy dependence of the diffusion coefficient can be derived from kinetic theory, where $D \approx \frac{1}{3} v_g \lambda$, with v_g being the quasiparticle group velocity and λ the mean free path. The group velocity is given by:

$$v_g = \frac{1}{\hbar} \frac{dE}{dk} = \frac{1}{\hbar} \frac{dE}{d\epsilon} \frac{d\epsilon}{dk} = \frac{\epsilon}{\hbar E} \frac{d}{dk} \left(\frac{p^2}{2m} \right) = \frac{\epsilon}{E} \frac{p}{m} = \frac{\sqrt{E^2 - \Delta^2}}{E} v_F, \quad (30)$$

where v_F is the Fermi velocity. Assuming the mean free path λ for quasiparticle scattering is approximately the same as in the normal state, the diffusion coefficient in the superconducting state, D_S , scales with the group velocity relative to the normal state:

$$D(E, \mathbf{r}) = D_0 \frac{v_g}{v_F} = D_0 \sqrt{1 - \left(\frac{\Delta(\mathbf{r})}{E} \right)^2}, \quad (31)$$

where D_0 is the diffusion coefficient in the normal state. This expression naturally incorporates the phenomenon of **quasiparticle trapping**: in a region where a quasiparticle's energy E is less than the local gap $\Delta(\mathbf{r})$, its group velocity and diffusion coefficient become imaginary, meaning it cannot propagate. Physically, we set $D(E, \mathbf{r}) = 0$ for $E < \Delta(\mathbf{r})$, trapping the quasiparticle.

4 Quasiparticle Dynamics: Numerical Simulation

To solve the full reaction-diffusion equation (Eq. 28), we employ a numerical approach based on the method of lines, discretizing both the spatial and energy domains. This allows us to model the behavior of the quasiparticle spectral density $n(E, \mathbf{r}, t)$ in time.

4.1 Discretization Scheme

We focus on a one-dimensional system, discretizing the spatial coordinate x into N_x pixels of width Δx , indexed by $k = 1, \dots, N_x$. The energy domain is discretized into N_E bins of constant width ΔE above the minimum gap Δ_{\min} , indexed by $i = 1, \dots, N_E$. The spectral density at a given time step m is thus represented by a matrix $n_{i,k}^m = n(E_i, x_k, t_m)$.

To solve the time evolution, we use **operator splitting**. In this approach, for each small time step Δt , we sequentially apply the effects of the diffusion operator and the collision operator.

1. **Collision Step:** For each spatial pixel k , we solve the master equation (the collision integral) for all energy bins i , updating the density from $n_{i,k}^m$ to an intermediate state $n_{i,k}^*$.
2. **Diffusion Step:** For each energy bin i , we solve the diffusion equation for all spatial pixels k , updating the density from the intermediate state $n_{i,k}^*$ to the final state at the next time step, $n_{i,k}^{m+1}$.

4.2 The Discretized Collision Integral

The collision integral $\mathcal{I}_{\text{coll}}[n]$ contains all local kinetic processes. At each spatial pixel k , its discretized form for the i -th energy bin is:

$$\begin{aligned} \mathcal{I}_{\text{coll}}[n_{i,k}] = & g_{\text{ext}}(E_i, x_k) + G_{\text{therm}}(E_i, x_k) \\ & + \Delta E \cdot \rho_{i,k} [1 - f_{i,k}] \sum_{j=1}^{N_E} n_{j,k} K_{ji,k}^s \\ & - n_{i,k} \Delta E \sum_{j=1}^{N_E} K_{ij,k}^s \rho_{j,k} [1 - f_{j,k}] \\ & - 2n_{i,k} \Delta E \sum_{j=1}^{N_E} K_{ij,k}^T n_{j,k}. \end{aligned} \quad (32)$$

Here, $\rho_{i,k} = \rho(E_i, x_k)$, $f_{i,k} = n_{i,k}/\rho_{i,k}$, and the kernels $K_{ij,k}^s = K^s(E_i, E_j)$ and $K_{ij,k}^r = K^r(E_i, E_j)$ are evaluated at the local gap $\Delta(x_k)$. This system of ordinary differential equations, $\partial n_{i,k}/\partial t = \mathcal{I}_{\text{coll}}[n_{i,k}]$, is typically stiff and is solved for one time step using an appropriate ODE solver (e.g., an implicit Runge-Kutta method).

4.3 The Discretized Diffusion Equation

The diffusion part of the evolution, $\partial n/\partial t = \nabla \cdot [D \nabla n]$, is solved using the **Crank-Nicolson scheme**, which is unconditionally stable and second-order accurate in both space and time. For a given energy slice i , the discretized equation is:

$$\frac{n_k^{m+1} - n_k^m}{\Delta t} = \frac{1}{2} (\mathcal{L}[n_k^{m+1}] + \mathcal{L}[n_k^m]), \quad (33)$$

where we have dropped the energy index i for clarity, and \mathcal{L} is the finite-difference representation of the spatial diffusion operator, $\nabla \cdot [D\nabla n]$. For a non-uniform diffusion coefficient $D_k = D(E_i, n_k, x_k)$, the operator is:

$$\mathcal{L}[n_k] = \frac{1}{\Delta x^2} \left[D_{k+\frac{1}{2}}(n_{k+1} - n_k) - D_{k-\frac{1}{2}}(n_k - n_{k-1}) \right], \quad (34)$$

with the diffusion coefficient evaluated at the pixel boundaries, e.g., $D_{k+\frac{1}{2}} = (D_{k+1} + D_k)/2$.

Rearranging the Crank-Nicolson equation groups the unknown terms at time step $m+1$ on the left and the known terms at time step m on the right, leading to a system of linear equations for the vector of spatial densities $\mathbf{n}^{m+1} = [n_1, n_2, \dots, n_{N_x}]^T$:

$$\mathbf{A}\mathbf{n}^{m+1} = \mathbf{B}\mathbf{n}^m. \quad (35)$$

The matrices \mathbf{A} and \mathbf{B} are tridiagonal and their elements are given by:

$$A_{k,k} = 1 + \frac{\Delta t}{2\Delta x^2}(D_{k+\frac{1}{2}} + D_{k-\frac{1}{2}}) \quad (36)$$

$$A_{k,k\pm 1} = -\frac{\Delta t}{2\Delta x^2}D_{k\pm\frac{1}{2}} \quad (37)$$

$$B_{k,k} = 1 - \frac{\Delta t}{2\Delta x^2}(D_{k+\frac{1}{2}} + D_{k-\frac{1}{2}}) \quad (38)$$

$$B_{k,k\pm 1} = \frac{\Delta t}{2\Delta x^2}D_{k\pm\frac{1}{2}} \quad (39)$$

This tridiagonal system can be solved very efficiently for each energy slice using standard algorithms like the Thomas algorithm.

A Numerical Methods and Implementation Details

This appendix provides a more detailed description of the numerical methods used to solve the full reaction-diffusion equation (Eq. 28), including specific algorithms, implementation strategies, and a formal analysis of the system's numerical properties.

A.1 Overall Algorithm Structure

The simulation solves the full dynamics by employing **operator splitting**, which separates the effects of diffusion and local collisions into distinct steps. The main simulation loop advances the system in discrete time steps Δt and follows this sequence:

1. **External Generation/Injection:** Add new quasiparticles to the density matrix $n_{i,k}$ from external sources g_{ext} , if applicable. This is typically a simple additive step.

2. **Collision Step:** For each spatial pixel k , solve the master equation (Eq. 18) for a duration Δt to account for all local kinetic processes (scattering, recombination, thermal generation). This updates the density from $n_{i,k}(t)$ to an intermediate state $n_{i,k}^*$.
3. **Diffusion Step:** For each energy bin i , solve the diffusion equation for a duration Δt to account for spatial transport. This updates the density from the intermediate state $n_{i,k}^*$ to the final state at the next time step, $n_{i,k}(t + \Delta t)$.
4. **Visualization/Data Storage:** Save or plot the state of the system as required.

The following sections detail the implementation of the collision and diffusion steps.

A.2 The Diffusion Step: Crank-Nicolson Method

The diffusion part of the evolution, $\partial n / \partial t = \nabla \cdot [D \nabla n]$, is handled using the **Crank-Nicolson scheme**. This method is implicit, unconditionally stable, and second-order accurate in both space and time. As shown in the main text, it results in a tridiagonal system of linear equations of the form $\mathbf{A} \mathbf{n}^{m+1} = \mathbf{B} \mathbf{n}^m$ for each energy slice.

A.2.1 The Thomas Algorithm for Tridiagonal Systems

This tridiagonal system can be solved very efficiently using the **Thomas algorithm**, a specialized form of Gaussian elimination that runs in $O(N_x)$ time, where N_x is the number of spatial pixels. For a system written as:

$$\begin{bmatrix} b_1 & c_1 & 0 & \cdots & 0 \\ a_2 & b_2 & c_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & b_{N_x} \end{bmatrix} \begin{bmatrix} n_1 \\ n_2 \\ \vdots \\ n_{N_x} \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ \vdots \\ d_{N_x} \end{bmatrix} \quad (40)$$

where the vector $\mathbf{d} = \mathbf{B} \mathbf{n}^m$ is the known right-hand side, the algorithm proceeds in two sweeps:

1. Forward elimination: The upper diagonal is eliminated by calculating modified coefficients:

$$c'_1 = \frac{c_1}{b_1} \quad (41)$$

$$c'_k = \frac{c_k}{b_k - a_k c'_{k-1}}, \quad k = 2, 3, \dots, N_x - 1 \quad (42)$$

$$d'_1 = \frac{d_1}{b_1} \quad (43)$$

$$d'_k = \frac{d_k - a_k d'_{k-1}}{b_k - a_k c'_{k-1}}, \quad k = 2, 3, \dots, N_x \quad (44)$$

2. Back substitution: The solution vector $\mathbf{n} = [n_1, \dots, n_{N_x}]^T$ is found:

$$n_{N_x} = d'_{N_x} \quad (45)$$

$$n_k = d'_k - c'_k n_{k+1}, \quad k = N_x - 1, N_x - 2, \dots, 1 \quad (46)$$

A.2.2 Boundary Conditions

Physical boundary conditions are implemented by modifying the first and last rows of the tridiagonal matrices \mathbf{A} and \mathbf{B} . For **insulating** (zero-flux) boundary conditions, we enforce $\partial n / \partial x = 0$ at the boundaries. For a forward-difference approximation at $x = 0$, this means $n_1 = n_2$, which can be enforced by adjusting the matrix elements $A_{1,1}, A_{1,2}, B_{1,1}, B_{1,2}$ accordingly to ensure no net flux.

A.2.3 Pre-computation for Efficiency

For a spatially varying but time-independent gap profile $\Delta(x)$, the diffusion coefficient $D(E_i, x_k)$ is also time-independent. Consequently, the matrices \mathbf{A} and \mathbf{B} and the Thomas algorithm forward-elimination factors (c'_k) are constant throughout the simulation for each energy slice. A significant computational speedup can be achieved by pre-calculating and storing these arrays in memory before the main simulation loop begins. The diffusion step then reduces to calculating the right-hand side vector \mathbf{d} and performing the back-substitution sweep at each time step.

A.3 The Collision Step: Time Integration

The collision step involves solving the system of coupled ordinary differential equations (ODEs) defined by the collision integral, $\partial n_{i,k} / \partial t = \mathcal{I}_{\text{coll}}[n_{i,k}]$, for each spatial pixel k .

A straightforward approach is to use an **explicit time-stepping** method, such as Forward Euler. In this scheme, the update rule for one time step Δt is simply:

$$n_i(t + \Delta t) = n_i(t) + \Delta t \cdot \mathcal{I}_{\text{coll}}[n_i(t)]. \quad (47)$$

While simple to implement, this method's stability is conditional on using a very small time step. A more rigorous analysis reveals that this is not an efficient approach for this particular physical system.

A.3.1 Numerical Stiffness and the Case for Implicit Solvers

A system of differential equations is considered **stiff** if it describes physical processes that occur on vastly different timescales. In our case:

- **Fast Processes:** High-energy quasiparticles ($E \gg \Delta$) rapidly lose energy by scattering with phonons, relaxing towards the gap edge.
- **Slow Processes:** Quasiparticles clustered near the gap edge ($E \approx \Delta$) are removed via two-body recombination, a much slower process, especially at low densities.

Using a standard *explicit* numerical solver (like Forward Euler) would require a time step smaller than the fastest timescale to maintain stability. To model the slow, long-term decay, this would be computationally prohibitive. *Implicit* solvers are designed to be stable even with large time steps, making them essential for stiff systems. We now estimate these timescales to demonstrate the system's stiffness.

The total rate at which a single quasiparticle at energy E scatters out is $\Gamma_{\text{scat}}(E) = 1/\tau_{\text{scat}}(E)$. For a high-energy quasiparticle ($E \gg \Delta$) emitting phonons at low temperature, we can approximate this rate:

$$\frac{1}{\tau_{\text{scat}}(E)} \approx \int_{\Delta}^E K^s(E, E') \rho(E') dE' \approx \int_{\Delta}^E \frac{1}{\tau_0} \frac{(E - E')^2}{(k_B T_c)^3} dE'. \quad (48)$$

Solving this integral gives an analytical estimate for the lifetime:

$$\tau_{\text{scat}}(E) \approx 3\tau_0 \left(\frac{k_B T_c}{E - \Delta} \right)^3. \quad (49)$$

Using typical parameters for aluminum ($\tau_0 \approx 400$ ns, $T_c \approx 1.2$ K, $\Delta \approx 180$ μeV , $k_B T_c \approx 103$ μeV), the lifetime for a quasiparticle at $E = 3\Delta$ is:

$$\tau_{\text{scat}}(3\Delta) \approx 3 \cdot (400 \text{ ns}) \left(\frac{103 \mu\text{eV}}{2 \cdot 180 \mu\text{eV}} \right)^3 \approx \mathbf{28 \text{ ns}}. \quad (50)$$

This establishes the fast timescale of the system.

Recombination is a two-body process, so its rate depends on the density of other quasiparticles. We consider the lifetime of a quasiparticle at the gap edge ($E \approx \Delta$) recombining with a bath of other quasiparticles also near the gap. The rate is:

$$\frac{1}{\tau_{\text{rec}}(E)} = 2 \int_{\Delta}^{\infty} K^r(E, E') n(E') dE'. \quad (51)$$

Approximating for $E, E' \rightarrow \Delta$, the kernel $K^r(\Delta, \Delta) \approx \frac{8\Delta^2}{\tau_0(k_B T_c)^3}$, and the integral $\int n(E') dE'$ becomes the density parameter x_{qp} . The recombination lifetime is therefore:

$$\tau_{\text{rec}} \approx \frac{\tau_0(k_B T_c)^3}{16\Delta^2} \frac{1}{x_{\text{qp}}}. \quad (52)$$

This is a key result: the lifetime is inversely proportional to the density. For a typical non-equilibrium density of $x_{\text{qp}}/(4N(0)) \sim 10^{-6}$, we find $x_{\text{qp}} \approx 9 \times 10^{-5}$ μeV , which gives a lifetime of $\tau_{\text{rec}} \approx \mathbf{9.3 \text{ ms}}$.

The ratio between the slow (recombination) and fast (scattering) timescales is $10^4 - 10^6$. This extreme separation confirms the system is numerically stiff. Therefore, despite the simplicity of an explicit method, a robust simulation requires an ****implicit ODE solver**** (e.g., an implicit Runge-Kutta method or a backward differentiation formula solver) for the collision step, as recommended in the main text.

A.3.2 Second-Order Decay Kinetics

The density-dependent lifetime is characteristic of a **second-order decay** process, which contrasts with the familiar first-order (exponential) decay.

- **First-Order:** The decay rate of a population N is proportional to N . The differential equation is $\frac{dN}{dt} = -\Gamma N$, which yields exponential decay, $N(t) = N_0 e^{-t/\tau}$. The lifetime $\tau = 1/\Gamma$ is constant.
- **Second-Order:** The decay rate is proportional to the rate of two-body encounters, i.e., N^2 . The differential equation is $\frac{dN}{dt} = -RN^2$, where R is a rate constant. This describes recombination. The solution is:

$$N(t) = \frac{N_0}{1 + RN_0 t} = \frac{N_0}{1 + t/\tau_0}, \quad (53)$$

where $\tau_0 = 1/(RN_0)$ is the initial lifetime. At long times, the population decays as $1/t$, which is much slower than exponential decay.

The slow, $1/t$ -like tail of the recombination process is a hallmark feature of quasiparticle dynamics.

A.4 Memory Layout and Data Structures

A practical implementation requires storing several large arrays. For a system with N_x spatial pixels and N_E energy bins, the primary data structures are:

- **Quasiparticle Density Array** $n_{k,i}$: A 2D array of size $N_x \times N_E$ holding the main dynamical variable.
- **Diffusion Coefficient Array** $D_{k,i}$: A 2D array of size $N_x \times N_E$ storing the diffusion coefficient for each energy at each location.
- **Thomas Algorithm Factors** $c'_{k,i}, d'_{k,i}$: 2D arrays of size $N_x \times N_E$ for the pre-computed factors of the diffusion solver.
- **Scattering and Recombination Kernels** $K_{k,i,j}^s, K_{k,i,j}^r$: 3D arrays of size $N_x \times N_E \times N_E$. These store the pre-computed values of the scattering and recombination kernels, which depend on the local gap $\Delta(x_k)$ and connect all pairs of energy bins (E_i, E_j) .

The memory required for the kernel arrays scales as $N_x N_E^2$ and often dominates the computational cost of the simulation.

References

- [1] John M. Martinis, M. Ansmann, and J. Aumentado. Energy Decay in Josephson Qubits from Non-equilibrium Quasiparticles. 2009. URL <https://arxiv.org/abs/0904.2171>.

- [2] M. Lenander, H. Wang, Radoslaw C. Bialczak, Erik Lucero, Matteo Mariantoni, M. Neeley, A. D. O'Connell, D. Sank, M. Weides, J. Wenner, T. Yamamoto, Y. Yin, J. Zhao, A. N. Cleland, and John M. Martinis. Measurement of energy decay in superconducting qubits from nonequilibrium quasiparticles. *Physical Review B*, 84(2), Jul 2011. ISSN 1550-235X. doi: 10.1103/physrevb.84.024501. URL <http://dx.doi.org/10.1103/PhysRevB.84.024501>.
- [3] J. Wenner and John M. Martinis. Erratum: Measurement of energy decay in superconducting qubits from nonequilibrium quasiparticles [Phys. Rev. B 84, 024501 (2011)]. Online, 2012. URL <https://web.physics.ucsb.edu/~martinisgroup/papers/Lenander2010erratum.pdf>. Accessed on 2023-10-27.