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Quasiparticles Density of States and the Scattering Rate in Ideal Type II Superconductor by a Time-Dependent Approach

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1. INTRODUCTION

The de Haas van Alphen (dHvA) effect in the vortex state of type II superconductors has been recently a rapidly developed field of research. Clear magnetization oscillations in the vortex state have been reported for half a dozen type-II superconducting (SC) materials of different types, such as the old high T_c, A-15 compounds [1], the new HTSC YBCO [2], the $(ET)_2Cu(NCS)_2$ organic superconductor [3], and the layered dichalcogenide $NbSe_2$ [4]. In all these experiments, the only observable effect of the SC order parameter on the measured magnetization oscillations, so far, has been an additional damping of the signal in the vortex state. Several theoretical attempts have been made to account quantitatively for this attenuation: Maniv *et al.* [5–9], Maki [10], Stephen [11–12], Dukan *et al.* [13–15], and Norman *et al.* [16–17]. Nonetheless, there is no complete quantitative theory yet that describes the magnetic oscillations behavior from the vicinity of the upper critical field deep into the mixed state far below the upper critical field.

In this note the quasiparticles density of states (DOS) of an ideal type II superconductor under strong magnetic field, and the scattering rate of the quasiparticles due to the appearance of the superconducting order parameter are studied by a converged quantum mechanical wave packet dynamic on a grid. The Chebychev propagation scheme [18–19], and other related methods are widely used to perform numerically converged quantum mechanical calculations in various areas of quantum molecular dynamics. Gorkov equation (see Eqs. (1a)–(1b) have the form of an inhomogeneous time-dependent Schrödinger equation. Hence, the powerful Chebychev propagation scheme, which provides an exact numerical solution to the time-dependent Schrödinger equation, can be applied to the Gorkov equation in order to obtain an exact numerical solution for this system. An important advantage of the Chebychev propagation scheme is its flexability. Different superconducting order parameters that might for example simulate a nonideal type-II superconductor, or a type-II superconductor with a low Ginzburg–Landau parameter in which the magnetic field has a strong spatial dependence, can be studied using the same computer code that is used in this publication for an ideal type-II superconductor under homogeneous magnetic field. Absorption of electromagnetic waves by the quasiparticles in the mixed superconducting state can be studied using the Chebychev propagation scheme.

The outline of this note is as follows: In Section 2 the solution Gorkov equation by the Chebychev propagation scheme is formulated. In Section 3 the numerical results are given and Section 4 concludes.

2. THEORY

The Gorkov formalism reduces the correlated BCS many-body problem in a mean field approximation to two coupled equations that involve only two time-ordered thermal Green's functions: a one particle many body Green's function and an anomalous Green's function. The latter is related to the superconducting order parameter (see Fetter and Walecka [20]). Gorkov differential equations for the time-ordered thermal Green's function are:

$$\begin{pmatrix} \hbar \dfrac{\partial}{\partial \tau} - \hat{H}_e & \Delta(\mathbf{r}) \\ \Delta^*(\mathbf{r}) & \hbar \dfrac{\partial}{\partial \tau} + \hat{H}_e^+ \end{pmatrix} \begin{pmatrix} G(\mathbf{r}, \tau, \mathbf{r}', \tau') \\ F^+(\mathbf{r}, \tau, \mathbf{r}', \tau') \end{pmatrix} = \begin{pmatrix} \hbar\delta(\mathbf{r} - \mathbf{r}')\delta(\tau - \tau') \\ 0 \end{pmatrix}. \tag{1a}$$

$\hat{H}_e$ is the Hamiltonian of a charged Fermion in the presence of the vector potential $\mathbf{A}$

$$\hat{H}_e = \frac{1}{2m}\left(-i\hbar\boldsymbol{\nabla} - \frac{q}{c}\mathbf{A}\right)^2 - E_F. \tag{1b}$$

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E_F is the Fermi energy and $\Delta(\mathbf{r}')$ is the superconducting order parameter which is related to the anomalous Green's function by the self-consistency condition $\Delta(\mathbf{r}') = \lambda F(\mathbf{r}, 0^+, \mathbf{r}, 0)$.

A converged time dependent quantum mechanical wave packet propagation on a grid by Chebychev polynomials expansion of the evolution operator (see Refs. [18–19]) is used to solve Gorkov equation in the time domain. The imaginary time, τ, that appears in Eq. (1a), is replaced by $-it$, and the time ordered thermal Green's function becomes a real time ordered Green's function from which the zero temperature properties can be obtained. A formal solution of the Gorkov equation can be written as

$$\begin{pmatrix} G(\mathbf{r}, t, \mathbf{r}', 0) \\ F^+(\mathbf{r}, t, \mathbf{r}', 0) \end{pmatrix} = \hat{U}(t) \begin{pmatrix} G(\mathbf{r}, 0, \mathbf{r}', 0) \\ F^+(\mathbf{r}, 0, \mathbf{r}', 0) \end{pmatrix}, \quad (2)$$

where $\hat{U}(t)$ is the evolution operator:

$$\hat{U}(t) = \exp\left\{ -i\frac{t}{\hbar} \begin{pmatrix} \hat{H}_e & \Delta(\mathbf{r}') \\ \Delta^*(\mathbf{r}') & -\hat{H}_e^* \end{pmatrix} \right\}. \quad (3)$$

$\Delta(\mathbf{r}')$ is taken as the Abrikosov vortex lattice [21], which is a self-consistent solution for the superconducting order parameter in the vicinity of the upper critical field $H_{c2}(T)$

$$\Delta(\mathbf{r}') = \Delta_0 \sum_j^{\infty} \exp\left(\frac{i2j\sqrt{\pi}x}{l}\right) \exp -\left(\frac{y}{l} + j\sqrt{\pi}\right)^2. \quad (4)$$

The magnetic length is $l = \sqrt{\hbar c/eH_0}$. The order parameter given in Eq. (4) describes an Abrikosov lattice with a quadratic unit cell, while a triangular Abrikosov lattice has a lower free energy and is the flux lattice found in type-II superconductors [22]. Note that the method presented here can be equally applied to Gorkov equation with a triangular flux lattice or any other form of a superconducting order parameter.

In the vicinity of $H_{c2}(T)$, $\Delta(\mathbf{r}')$ is small. Thus the initial Green's function can be approximated by the Green's function of a normal electron gas in a uniform magnetic field

$$-iG(\mathbf{r}, 0^+, \mathbf{r}', 0') = \sum_{n=n_F-n_D}^{n_F+n_D} \sum_{k_x} \phi_n^{k_x}(x, y)\phi_n^{k_x *}(x', y'), \quad (5)$$

with $n_F = E_F/\hbar\omega_c$, $n_D = \omega_D/\omega_c$, and

$$\phi_n^{k_x}(x, y) = \sqrt{1/L^2 2^n n! \sqrt{\pi} l}\, e^{-ik_x x}\, e^{-(1/2)(\frac{y}{l}+k_x l)^2} H_n\left(\frac{y}{l} + k_x l\right). \quad (6)$$

$\phi_n^{k_x}(x, y)$ are eigenfunctions of the Hamiltonian for a single electron in a uniform magnetic field in the Landau gauge. A cutoff at the Debye frequency, $\hbar\omega_D$, measured from the Fermi energy is introduced into the initial Green's function by restricting the sum over Landau levels in Eq. (5) to

$$n_F - \frac{\omega_D}{\omega_c} < n < n_F + \frac{\omega_D}{\omega_c}. \quad (7)$$

The anomalous Green's function, $F^+(\mathbf{r}, 0, \mathbf{r}, 0)$, is taken to be identically zero at $t = 0$ since this is the limit of a free electron gas in a uniform magnetic field with no superconducting order. The initial spinoric wave packet evolves into the wave packets at time t by the operation of the time evolution operator (Eq. (3)), and in terms of the Chebychev propagation scheme (see Refs. [18–19]) is given by

$$\begin{pmatrix} G(\mathbf{r}, t, \mathbf{r}', 0) \\ F^+(\mathbf{r}, t, \mathbf{r}', 0) \end{pmatrix} = \sum_n A_n(\alpha) \begin{pmatrix} \phi_{+_n}(\mathbf{r}) \\ \phi_{-_n}(\mathbf{r}) \end{pmatrix}, \quad (8)$$

where $\alpha = \Delta E t/\hbar$ and $A_n(\alpha)$ is $2 \times J_n(\alpha)$ (J_n is a Bessel function of the first kind) and $A_0(\alpha)$ is $J_0(\alpha)$. The spinor, $\binom{\phi_{+n}(\mathbf{r})}{\phi_{-n}(\mathbf{r})}$, is calculated by the Chebychev recursion formula during the propagation:

$$\begin{pmatrix} \phi_{+_{n+1}}(\mathbf{r}) \\ \phi_{-_{n+1}}(\mathbf{r}) \end{pmatrix} = \frac{2i}{\Delta E} \begin{pmatrix} \hat{H}_e & \Delta(\mathbf{r}) \\ \Delta(\mathbf{r})^* & -\hat{H}_e^* \end{pmatrix} \begin{pmatrix} \phi_{+_n}(\mathbf{r}) \\ \phi_{-_n}(\mathbf{r}) \end{pmatrix} - \begin{pmatrix} \phi_{+_{n-1}}(\mathbf{r}) \\ \phi_{-_{n-1}}(\mathbf{r}) \end{pmatrix}. \quad (9)$$

ΔE is an energy interval that normalizes the eigenvalues of the system to the range $[-1, 1]$, where the Chebychev polynomials are defined.

The Fourier transform of the propagated wave packet at the point $\mathbf{r} = \mathbf{r}'$ is calculated as follows: During the propagation a vector $\mathbf{P}$, that is defined below is computed and stored. The one point Green's function as a function of time is given in terms of the vector components by

$$G(\mathbf{r}, t, \mathbf{r}, 0') = \sum_n A_n(\alpha) P_n \quad (10a)$$

$$P_n = \phi_{+_n}(\mathbf{r}). \quad (10b)$$

The index n denotes the nth Chebychev polynomial used in the calculation. A convergence of the sum is reached when n is greater than α. This is due to the exponential decay of a Bessel function when its order is greater than its argument. The Fourier transform was calculated analytically [19] and is given by

$$G(\mathbf{r}, \mathbf{r}, \omega) = \sum_n c_n(\beta) P_n \quad (11a)$$

where

$$c_0(\beta) = \frac{2}{\sqrt{1-\beta^2}} \tag{11b}$$

$$\beta = \frac{\hbar\omega}{\Delta E} \tag{11c}$$

$$c_n(\beta) = \begin{cases} \dfrac{4\cos(n\sin^{-1}(\beta))}{\sqrt{1-\beta^2}} & \text{if } n \text{ is even} \\ \dfrac{4\sin(n\sin^{-1}(\beta))}{\sqrt{1-\beta^2}} & \text{if } n \text{ is odd.} \end{cases} \tag{11d}$$

Local density of states can be calculated as the imaginary part of the one point Green's function $\mathbf{r}' = \mathbf{r}$

$$N(\mathbf{r}, \omega) = -\frac{1}{\pi}\,\mathrm{Im}(G(\mathbf{r}, \mathbf{r}, \omega)). \tag{12}$$

3. NUMERICAL RESULTS

a. *Quasiparticles Density of States in the Superconducting Mixed State*

The quasiparticles density of states (DOS) are shown in Figs. 1a–b with $\Delta_0 = 0.5$ and $1.0\hbar\omega_c$ accordingly, where $E_F = (n_f + \frac{1}{2})\hbar\omega_c$, $n_f = 25$, such that Fermi energy coincides with the 25th Landau level. The DOS splits into a few subbands with a mirror symmetry around $E = 0$ due to the symmetry of the BdG equations [23]. The positive energy subband in Fig. 1a is the quasiparticle excitation energies (whereas the mirror image negative energy subband corresponds to the energy gained by the destruction of a quasiparticle). The maximal weight of the DOS is shifted to a positive energy by the appearance of the superconducting order parameter, $\Delta(\mathbf{r})$. The shift of the DOS to positive energies is a growing function of the SC order parameter Δ_0, as shown in Figs. 1a–b. The quasiparticle DOS depends strongly on the position of the Fermi energy with respect to a Landau level. In Figs. 2a–e the Fermi energy is varied from $(25 + \frac{1}{2} - 0.5)\hbar\omega_c$ up to $(25 + \frac{1}{2} + 0.4)\hbar\omega_c$ by steps of $0.2\hbar\omega_c$; $\Delta_0 = 1.0\hbar\omega_c$ in all figures. When the Fermi energy coincides with a Landau level the DOS maximum is close to $E = 0$ as seen in Fig. 2c with $E_F = (25 + \frac{1}{2})\hbar\omega_c$, but the peak of the DOS does not coincide with $E = 0$ due to the presence of the SC order paramter. For smaller and larger values of Fermi energy, $25.1\hbar\omega_c$, $25.3\hbar\omega_c$ and $25.7\hbar\omega_c$, $25.9\hbar\omega_c$ the DOS maximum is gradually shifted further away from the origin of the quasiparticles spectrum at $E = 0$. The dependence pattern of the DOS on the position of the Fermi energy with respect to a Landau level seen in Figs. 2a–e repeats itself for each Landau level. Two characteristics of the magnetization oscillations observed in type-II superconductors under strong magnetic fields can be deduced from analyzing Figs. 1a–b and 2a–e. First, the magnetization oscillations are expected to persist in the SC state (in type-II SC) with the same period as in the normal state since the quasiparticles DOS shows a periodic behavior with respect to Landau levels. Second, the magnetization oscillations amplitude is expected to be additionally damped in the SC state due to the reduction and the different pattern of the quasiparticles DOS at Fermi energy with respect to the DOS of a free electrons gas.

b. *The Scattering Rate in the Superconducting Mixed State*

In Fig. 3 the absolute value of the Green's function is shown. There are three time scales that characterize the behavior of the Green's function at short propagation times in a similar way to the behavior of the autocorrelation function found by Heller [24] and by Rom *et al.* [25]. The shortest time scale, τ_1, determined by the half-width half-maximum of a recursion peak, is related to the broadest feature in the energy domain which is the Debye cutoff energy. The second time scale, τ_2, is the time separation between the recursion peaks and is related to the Landau energy spacing, $\omega_c = 2\pi/\tau_2$. The third time scale, τ_3, is determined by the Gaussian envelope created by the maxima of the recursion peaks. τ_3 is a relaxation time related to the broadening of Landau levels.

The Gaussian envelope obtained in the time domain indicates a Gaussian broadening envelop of the DOS in the energy domain which means a short tail of eigenvalues measured from an unperturbed Landau level and a clear magnetic gap between adjacent Landau levels for relatively big values of Δ_0.

In a plot of $-\ln|G(\mathbf{r}, \mathbf{r}, t)/G(\mathbf{r}, \mathbf{r}, 0)|$ vs t^2 the recursion peaks seen in Fig. 3 appear as a set of minima at each recursion. If Green's function has a Gaussian envelope, a straight line can connect the minima. The slope of the line is $1/\tau_3^2$, where τ_3 is the characteristic relaxation time, and $1/\tau_3$ is the scattering rate of the quasiparticles in the superconducting state. The dependence of the scattering rate on th value of Δ_0 is found numerically to be linear for small values of $\Delta_0(\sim\hbar\omega_c)$, and is given by

$$\frac{\pi}{\tau_3\omega_c} = 0.2096\,\frac{\Delta_0}{\hbar\omega_c}. \tag{13}$$

The small numerical prefactor, 0.2096, combined with the Gaussian envelope of the density of states means that Δ_0 can get large values, in units of the Landau energy levels spacing $\hbar\omega_c$, before a strong overlap of the Landau levels will be seen.

The dependence of the scattering rate, $1/\tau_3$, on n_F is nonmonotonic but follows a decreasing envelope. The

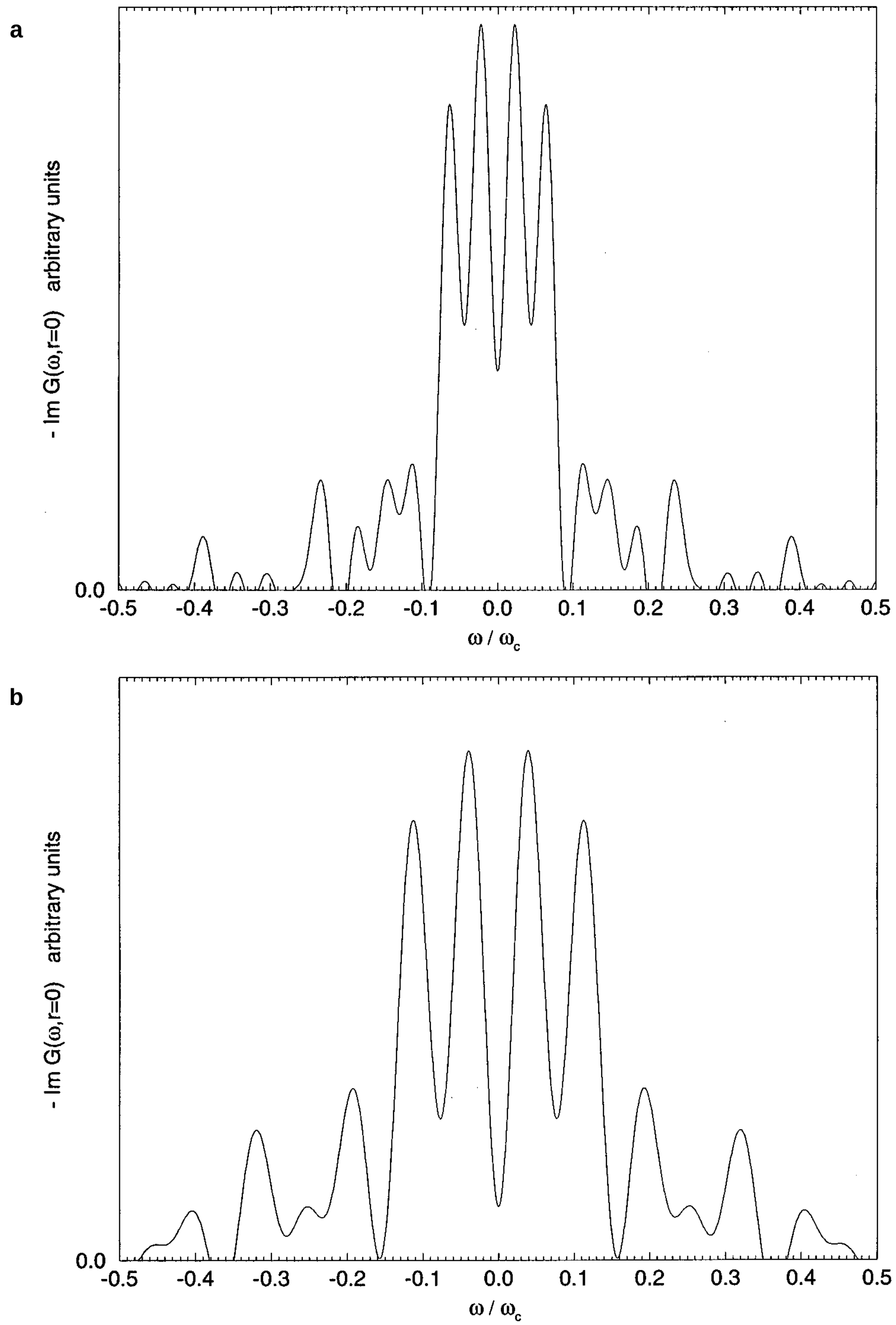

FIG. 1. Quasiparticles density of states calculated by the Chebychev propagation scheme with $n_f = 25$, $\Delta_0 = 0.5\hbar\omega_c$ in (a) and $1.0\hbar\omega_c$ in (b).

decreasing envelope is approximated by the curve $0.475 n_F^{-1/4}$. The dependence of the relaxation time on $\ln(n_D)$, where the Debye cutoff is $\hbar\omega_D = n_D\hbar\omega_c$, is found to be linear; thus the relaxation time, τ_3, depends logarithmically on the Debye cutoff. To summarize, our numerical results show that the scattering rate, $1/\tau_3$, with τ_3 determined by the Gaussian envelope of the one point Green's function in the time domain, depends linearly on Δ_0 and λ and has an inverse dependence on n_F with a small power of $\frac{1}{4}$:

$$\frac{1}{\tau_3} \sim \lambda\Delta_0 n_F^{-1/4}. \tag{14}$$

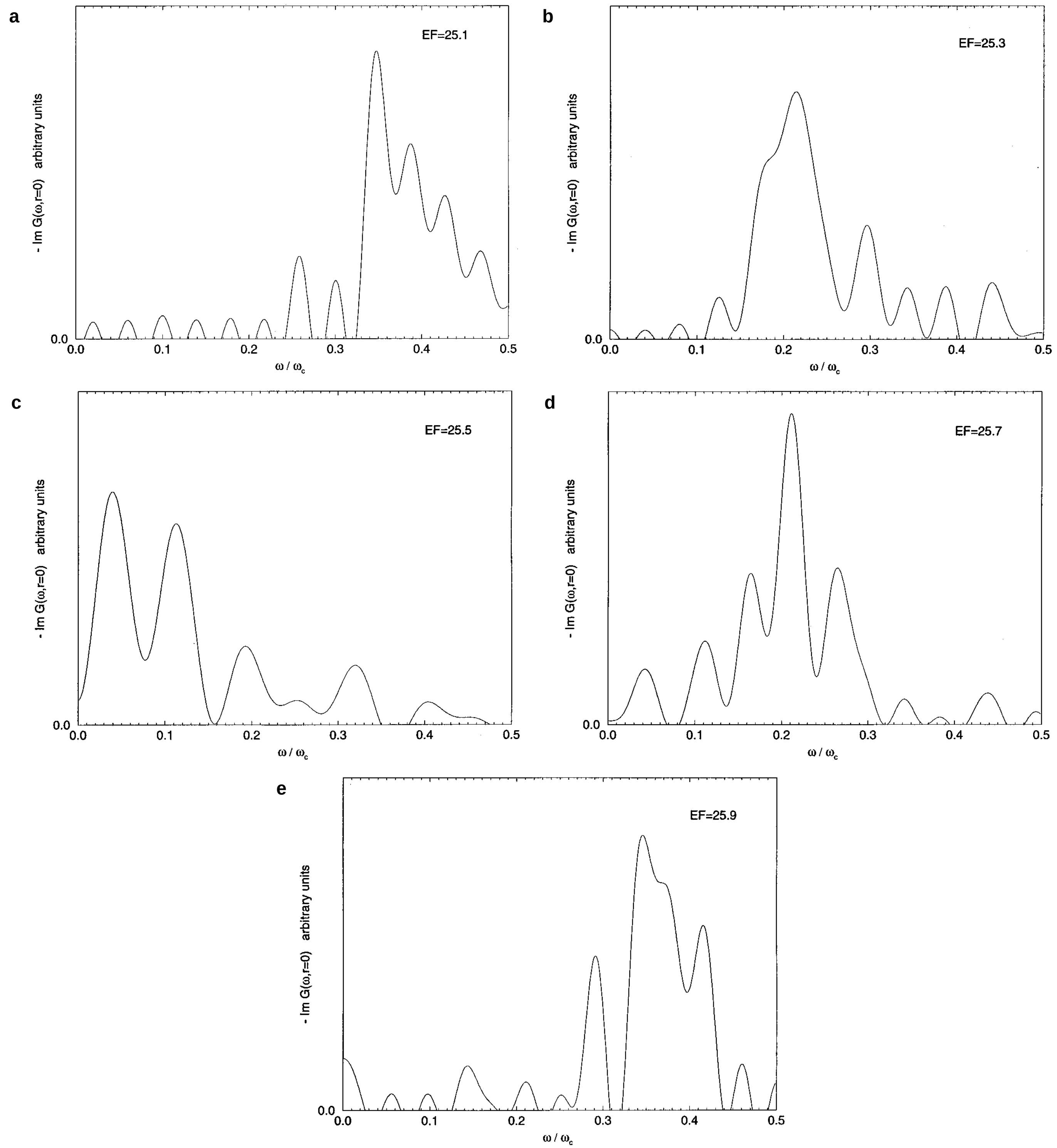

FIG. 2. Quasiparticles density of states dependence on Fermi energy. The Fermi energy is varied from $(25 + \frac{1}{2} - 0.4)\hbar\omega_c$ in (a) up to $(25 + \frac{1}{2} + 0.4)\hbar\omega_c$ in (e) by steps of $0.2\hbar\omega_c$. $\Delta_0 = 1.0\hbar\omega_c$ in all figures.

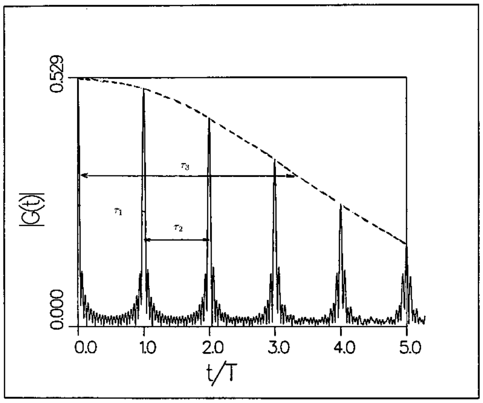

FIG. 3. The absolute value of the one point Green's function in five periods, showing the Gaussian envelope and the three time scales τ_1, τ_2, and τ_3; $n_F = 25$; $n_D = 11$; $\Delta_0 = 0.5\hbar\omega_c$.

This result, for the scattering rate dependence on the various parameters, is in agreement with the expression for the scattering rate given by Norman *et al.* [17].

The Debye cutoff energy which is a fundamental quantity in the BCS theory for superconductivity [26] has a direct fingerprint in the evolution of Green's function in the time domain. It is related to the shortest time scale, τ_1, the half width half maximum of a recursion peak. Due to the Fourier relation between the time and energy domains, the shortest time scale in the time domain is related to the broadest energy scale, which is in this system the Debye cutoff energy. The dependence of τ_1 on the Debye cutoff energy, where the Debye cutoff is $\hbar\omega_D = n_D\hbar\omega_c$, is found to be linear in $1/n_D$ and is given by

$$\frac{\tau_1\omega_c}{2\pi} = 0.271\frac{1}{n_D}. \tag{15}$$

4. CONCLUSION

In this note a time-dependent approach to Gorkov equation based on the Chebychev propagation scheme was presented. The time-dependent wave-packet propagation on grid approach used here is very flexible and can be used to study for example nonideal type-II superconductors, SC with low Gizburg–Landau parameter and absorption of electromagnetic waves by quasiparticles in the mixed state. The basis set approaches [11, 13–15, 16–17] use the explicit form of Abrikosov SC order parameter with a particular set of functions (magnetic Bloch functions) to calculate analytically the BdG Hamiltonian matrix elements. These approaches are very efficient but not flexible since if a different form of a SC order parameter needs to be considered, the matrix elements have to be recalculated and are not expected to be analytic for a nonideal superconductor.

The quasiparticles density of states dependence on the order parameter amplitude, Δ_0, and on the Fermi energy was studied. The DOS maximum is shifted to a positive value and a deep hole in the middle of the highest occupied Landau level is seen. Since the quasiparticles DOS in the SC state have a different pattern at the Fermi energy than the DOS of a free electrons gas, and due to the fact that the quasiparticles DOS is not peaked at the Fermi energy when the latter coincides with a Landau level, the magnetization oscillations amplitude is expected to be dampled faster in the SC state.

It is found that the envelope of the local (one point) electron Green's function at short times is Gaussian. From the envelope a scattering rate, which is related to the broadening of Landau levels, is extracted. The scattering rate depends logarithmically on the Debye cutoff energy, linearly on the superconducting order parameter Δ_0 and is proportional to a small negative power of the filling factor, i.e., $n_F^{-1/4}$, where $n_F = E_F/\hbar\omega_c$.

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