Non-equilibrium local pair potential enhancement

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We propose a new nonequilibrium mechanism for the local pair potential enhancement with the help of electromagnetic control fields. The mechanism is based on the creation of non-equilibrium, spatially localized Bogoliubov quasiparticle excitations, which result in a significant enhancement of the local pair potential and the local transition temperature \(T_c\).

A properly cooled Fermi atomic gas with an attractive interaction between atoms can undergo a superfluid transition analogous to the BCS transition in superconductors \([1]\). This theoretical prediction motivated many experiments to study the superfluid properties of cold Fermi systems \([2, 3]\) along with additional theoretical work (see, for example, \([4]\) and the references therein). Experimental studies have been carried out on the manipulation of cold Fermi gases \([5]\) based on the control of the critical transition temperature \(T_c\). Control has been achieved by application of an external magnetic field \([5, 6]\), which can modify the effective interaction between atoms due to the Feshbach resonance \([6]\). The enhanced interatomic interaction may produce a stronger pairing potential and a higher \(T_c\).

In this work we propose a new nonequilibrium mechanism for pair potential enhancement, which is not based on the direct control of the effective interaction between fermions, but rather relies on control of the spatial localization of the quasiparticle density in the system. The local pair potential \(\Delta(x_0, t_0)\) at a given position \(x_0\) and time \(t_0\) is proportional to the product of the local amplitudes of the quasi-electron and quasi-hole (Bogoliubov) excitations \(\psi^\ast(x_0, t_0)\psi(x_0, t_0)\) \([6]\). If an external control field is chosen in a such way that it drives a significant amount of the quasiparticles to be localized at a certain moment in the vicinity of \(x_0\), this can lead to an enhancement of the local pair potential \(\Delta(x_0, t_0)\). Therefore, the pair potential can be enhanced locally in a target volume rather than in the whole system, and this enhancement is achieved along with decreasing of the quasiparticles density and the local pair potential elsewhere. This will in effect, result in increase of the local effective critical transition temperature \(T_c(x_0, t_0)\). A simple estimate of the enhancement of the transition temperature at a given moment \(t_0\) can be obtained using the BCS expression for bulk superconductors \(T_c(x_0, t_0) \approx \Delta(x_0, t_0)/(1.76k_B)\).

The suggested mechanism should be contrasted with the known Eliashberg mechanism of the pair potential enhancement in superconductors \([8]\). Since the time-dependent electromagnetic field may create a nonequilibrium distribution of quasiparticles in the superconductor, it may lead to unoccupied states at the Fermi surface at the gap edge that effectively increases the gap value. However, the Eliashberg mechanism does not result in a spatially localized enhancement of the quasiparticle density. The Eliashberg mechanism is rather weak effect, resulting in a relative increase of the transition temperature \(T_c\) by an order of \(1\%\), and it was observed and extensively studied in the cases of electromagnetic, acoustic or tunneling processes \([9]\).

To illustrate our approach, let us consider the interaction a cold atomic Fermi gas with a time dependent control field. A nonequilibrium state of the system is described utilizing time-dependent Bogoliubov-de Gennes (TDBdG) equations for an inhomogeneous system \([7]\):

\[
i\hbar \frac{\partial u_n(r, t)}{\partial t} = H u_n(r, t) + \Delta(r, t)v_n(r, t), \quad (1)
\]

\[
i\hbar \frac{\partial v_n(r, t)}{\partial t} = -H v_n(r, t) + \Delta^\ast(r, t)u_n(r, t),
\]

with \(H = H_0 + U(r, t) + V(r, t) - \mu\), \(H_0\) defined by

\[
H_0 = -\frac{\hbar^2}{2m} \nabla^2 + W(r).
\]

Here \(m\) is electron mass, \(\mu\) is the chemical potential, \(W(r)\) is an external trapping potential, and \(V(r, t)\) is the control field. \(U(r, t)\) is the Hartree-like mean field local potential, given by

\[
U(r, t) = -D_0 \sum_n \{ |u_n(r, t)|^2 f_n + |v_n(r, t)|^2 (1 - f_n) \}.
\]

And \(\Delta(r, t)\) is the quantity of our interest: the local pair potential, which is

\[
\Delta(r, t) = D_0 \sum_n u_n(r, t)v_n^\ast(r, t)(1 - 2f_n).
\]

Here \(D_0\) is the effective attraction interaction coefficient. For example, for isotropic attractive interactions between neutral atoms in a trap \(D_0 = 4\pi\hbar^2/ma_s\), where \(a_s\) is the atomic scattering length.

To illustrate our approach let us consider a system consisting of a cooled atomic Fermi gas trapped in a potential...
In this case the potential is proportional to the time average of the local laser intensity $I(r)$. The intensity of laser can be modulated, which is equivalent to adding a time-dependent external control potential $V(r,t)$. For simplicity we assumed that the system is elongated and that the control field $-\nabla V(r,t)$ is linearly polarized along the same direction. Thus, the one dimensional description is adequate. For simplicity we set the trapping potential $W(x)$ to be a square well of the length $L$ with infinite walls. However, the suggested control strategy will work for other types of anharmonic trapping potentials with non equidistant transition frequencies. The system is assumed to be initially in the ground state. We used a mesh with $m = 16$ and $m = 32$ equidistant discretization points for the spatial variable to perform numerical integration of Eq. (1). We test our numerical routine by calculating the interaction of a resonant field with a single particle in an infinite square well potential and compared with the analytical solution for the Rabi oscillations between two different states. We found an excellent agreement between numerical and analytical solutions.

Optimal control of the local pair potential we formulate as a search for a field $V(x,t)$, which maximizes the average value of the pair potential $<\Delta >$ in a target area $[x_0 - \epsilon_0, x_0 + \epsilon_0]$ over a given time interval $t_0$:

$$<\Delta > = (2t_0\epsilon_0)^{-1} \int_{t_0}^{T} \int_{x_0-\epsilon_0}^{x_0+\epsilon_0} |\Delta(x,t)| dx dt.$$  \hspace{1cm} (5)

In order to understand how one can control the quantity $\Delta(x,t)$, we do the following analysis. The TDBdG equations Eq. (1) can be approximately solved in the absence of the control field $(V(x,t) = 0)$, assuming constant pair $\Delta(x) = \Delta_0$ and Hartree $U(x) = U_0$ potentials. The solution in this case is

$$u_n(x,t) \approx \bar{u}_n \psi_n(x)e^{-i\bar{E}_n t}, \quad v_n(x,t) \approx \bar{v}_n \psi_n(x)e^{-i\bar{E}_n t}.$$ \hspace{1cm} (6)

with $\bar{u}_n^2 = \frac{1}{2} \left( 1 + \frac{\epsilon_n - \bar{\mu}}{\bar{E}_n} \right), \quad \bar{v}_n^2 = \frac{1}{2} \left( 1 - \frac{\epsilon_n - \bar{\mu}}{\bar{E}_n} \right)$, where $\bar{\mu} = \mu - U_0$. The eigenenergies are $E_n = \sqrt{(\epsilon_n - \bar{\mu})^2 + \Delta_0^2}$, where $\epsilon_n$ and $\psi_n(x)$ are the eigenenergies and eigenfunctions for the stationary Schrödinger equation with the Hamiltonian Eq. (2). A control field that maximizes $<\Delta >$ should drive at least some of the amplitudes $u_n, v_n$ from their initial state $u_n(x,0), v_n(x,0)$ to a nonequilibrium state at the target time $u_n(x,T), v_n(x,T)$ (assuming $t_0 \ll T$), which will have a “bump” at, or in close vicinity of $x_0$.

As an initial guess for the control field $V(x,t)$ we choose one that drives the initial quasiparticle wavefunctions with the lowest energy $E_1, u_1(x,0), v_1(x,0)$, to a nonequilibrium localized state $u_1(x,T), v_1(x,T) \propto g(x)$, where $g(x) = (x - x_0)e^{-(x-x_0)^2/\alpha^2}$, which has two maximums near $x_0 = L/2$. The analytical solution for this optimal control field in the dipole approximation can be written using the results for localization of a particle in an infinite well potential obtained in \[10\]:

$$f(t) = \sum_{n=2,4,...} N_n \cos(\omega_n t/\hbar).$$ \hspace{1cm} (7)

where $\hbar \omega_n = E_n - E_1$, $\omega_n = \frac{\hbar \omega_n}{\hbar}$, $N_n = \int g(x)\psi_n(x)dx$ are the expansion coefficients for the target nonequilibrium state $g(x)$ in the basis $\psi_n(x)$, and $d_n = \int \psi_1(x)\psi_n(x)dx$ are the corresponding transition dipole matrix elements. For symmetric trapping potentials $W(x)$ the dipole matrix elements $d_n = 0$ if $n$ is odd, therefore we have chosen the target state $g(x)$ to be an antisymmetric function with respect to $x_0$. For an infinite well potential $\epsilon_n = \frac{h^2 x_0^2}{2mL^2}$, and the matrix elements can be also calculated analytically for even values of $n$: $d_n = -4L\cos(\pi n)n + n)/\pi(1 - n^2 + n^4)$. The expansion coefficients in the limit of small width of the target state $\alpha \ll L$, asymptotically approach $a_n = \sqrt{\pi}n^3 e^{-a^2(1 + \pi^2 n^2)^2}/(1 + \exp(\alpha^2 n)(n - 1) + n)/4$.

In the present calculations we have chosen $D_0 = 10^{-3}E_0$. The initial states $u_n(x,0), v_n(x,0)$ were not calculated self-consistently, instead we used the approximate analytical solution Eq. (6). The first six terms in Eq. (7) are used as a starting approximation for the control field. We assumed $\alpha = 0.1L$ and set the control time interval $T = 50\pi T_1$, where $T_1 = \frac{2\pi}{\bar{\mu}} = \frac{4\hbar^2 L^2}{\pi} \hbar^2$ is the time period for a particle occupying the ground state of an infinite well potential. For this relatively long control interval the amplitude a quasiparticle, which occupies the ground state of the potential will make about 150 oscillations. Therefore, the Rotating Wave Approximation, used in the derivation of Eq. (7) in \[10\] is justified. The optimal control will result in relatively slow Rabi oscillations of the occupation numbers $|a_n(t)|^2 \approx |a_n|^2 \sin^2(\frac{\pi t}{T_1})$, $n > 1 \[10\]$, where $a_n(t) = \int u_1(x,t)\psi_n(x)dx$. Similar dynamics can be observed for the quasi-holes $b_n(t) = \int v_1(x,t)\psi_n(x)dx$.

The amplitudes $V_n$ and the frequencies $\omega_n$ of the control field were used as an initial input for a black box optimization using simulated annealing algorithm. As the fitness function for the optimization we used the averaged pair potential Eq. (4) on the spatial interval $[L/2 - \epsilon_0, L/2 + \epsilon_0]$, with $\epsilon_0 = 0.1L$, and $t_0 = 0.1T$. The simulated annealing optimization resulted in additional $\approx 15\%$ improvement of the averaged magnitude of the pair potential $<\Delta >$ with respect to the enhancement, obtained using the non-optimized analytical solution Eq. (7). To reduce the amount of the meshing points we set the renormalized chemical potential $\bar{\mu}$ to zero, therefore limiting the amount of the nodes in the initial quasiparticle amplitudes. We considered the evolution of maximum 6 (3 quasi-electron, and 3 quasi-hole).
quasi particles. Such a small number was chosen because the characteristic single particle frequencies in a square well potential grow quickly (as \( n^2 \)) that makes numerical integration of TDDbG equations extremely slow. The resulting nonequilibrium dynamics of the pair potential \( |\Delta(x, t)| \) is shown in Fig.1. Note we assumed zero temperature. In Fig.1(a) one can see the gradual spatial localization of the pair potential near the center of the infinite well potential \( x_0 = L/2 \), which occurs at the end of the control interval. The local enhancement of the pair potential and the transition temperature \( T_c(x_0, T) \approx \Delta(x_0, T) \) is about 300\% compared to the initial state. In Fig.1(a) one can see that the enhancement is achieved at the price of decrease of the \( |\Delta(x, t)| \) outside the target area, closer to the walls of the trapping potential. In Fig.1 (b,c) we have shown similar simulations for optimal control of four and six quasiparticles, and the resulting dynamics of the pair potential. As in the case of just two quasiparticles, the pair potential shows a strong enhancement near the center of the well.

Note, the control field \( V(x, t) \) also drives other quasiparticle amplitudes \( u_n(x, T), v_n(x, T) \) with \( n > 1 \), but this does not change much the localization picture. One has to note that the enhancement is relatively weaker in the latter two cases shown in Fig.1 (b,c). The approximate analytical solution for the amplitudes \( a_n(t) \) and \( b_n(t) \) has the period of \( 4T \), therefore, for the controlled system \( |a_n(t)|^2 \) and \( |b_n(t)|^2 \) will return to their initial states at \( t = 2T \). In real systems this return will never be perfect, and it will correspond to the loss of coherence in the driven system and the energy dissipation. For strongly interacting quasiparticles the driven dynamics can significantly depart from the approximate analytical solution. In superconducting materials the pair potential \( \Delta \) is relatively small compared to the Fermi energy, and can be treated as a perturbation. However, this is not always the case, for example, in cold atomic Fermi gases. Relatively strong coupling between functions \( u_n \) and \( v_n \) in the presence of oscillatory field may lead to chaotic dynamics. In this case numerically stable control techniques of chaos are necessary.

The proposed mechanism may be applied not only to cold atomic Fermi gases, but also in solid state quasi-one dimensional superconducting systems. However, the thickness of the system should not be too small, since the gap enhancement can be suppressed by the phase slip phenomena [12], which is not included in our mean field description. One may consider an experiment with quasi one dimensional superconductors, such as a nanowire or a bundle of doped carbon nanotubes [14]. One may design an optimal control experiment, when the quantity of interest will be non-equilibrium conductivity of the bundle at a temperature close to \( T_c \). Making analogy with the Eliashberg effect [15], one may expect that a nonequilibrium perturbation of the system may increase the effective critical temperature (as well as the instantaneous pairing potential). Using an optimal control field one may drive periodically the quasiparticle density to be maximal along the bundle near its center, that will result in a considerable drop of the resistance of the bundle at times of the spatial localization. In order to achieve this, the control field should have its polarization, which is transverse to the bundle.

The control field Eq.(7) can be used in the experiment as an initial guess. Then one may use the mean-
sured nonequilibrium conductivity of the bundle at the target moment $T$ as a fitness function, in a similar fashion we used Eq. 4 for the simulated annealing optimization. Let us consider a bundle of boron or alkali-atoms doped carbon nanotubes of width $L = 500\text{nm}$ [14]. We assume the level of doping such that the carriers are having the wavelength of the order of 4 nm. As the initial guess for the control field we may choose a field that drives the initial quasiparticle wavefunction with the lowest energy $u_n(x) = u_{250} \propto \sin(250\pi x/L)$ to the target $v_{250}(x, T) \approx u_n(x, 0)g(x)$, where the function $g(x)$ is defined above. Note the control will be performed rather over the envelope of the quasiparticle wavefunctions. At the time $T$ the target wavefunction can be represented as $u_{250}(x, T) = \sum_{n=1}^{3} \sum_{j=250}^{250} a_n u_n(x, 0)$. The expansion coefficients of the target wavepacket $a_n$ can be used in the solution Eq. (7). The same control is applicable for the quasi-hole wavefunction $v_{250}(x)$. Even for a relatively modest density localization with $\alpha = 0.3L$ for just one pair of quasiparticles with the lowest energy, it will correspond to $\approx 300\%$ increase of the term $v_{250}u_{250}$ and the overall local increase of the pairing potential by $\approx 1\%$. One can use the adaptive optimization approach to further improve the localization of quasiparticles [16]. There may be some possible obstacles for the proposed experiment. First, relatively strong control field may result in strong energy dissipation. At the same time the control field can not be too weak, since it will increase the duration of the optimal control interval $T$. The duration of the control interval should not be too long, because the loss of coherence, for example, due to collisions of cold atoms, may reduce the efficiency of the proposed scheme [17].

To conclude, we presented a new approach to control the local enhancement of the pair potential. The enhancement is achieved through a nonequilibrium spatial localization of the quasiparticle density in the system. This mechanism contrasts with the spatially homogeneous Eliashberg mechanism, which usually employs a field with only a single frequency. Our method is based on coherent control, which requires a multi-frequency field with independently tuned field amplitudes. The suggested control scheme will be effective on the time scale, shorter than the effective decoherence times, which for Fermi gases can be of the order of milliseconds. The time-dependent Eq. (1) is valid for weakly nonequilibrium conditions, since $\Delta(\mathbf{r} , t)$ is defined by using the equilibrium values of the Fermi distribution $f_n$. Most significant, the electromagnetic field should not have components with the frequencies over the double gap size, $\hbar \omega_{\text{max}} > 2|\Delta|$, because high energy photons can easily break Cooper pairs. Assuming the equilibrium pairing potential $\Delta \approx 0.0015\text{eV}$ in the above described example with the bundle of doped carbon nanotubes, one may estimate that the transition frequencies between the nearest levels at the Fermi surface (assuming the infinite well potential model) will be about $\Delta E \approx 0.0007\text{eV}$. Therefore operating with a radio frequency field with $\hbar \omega_{\text{max}} < 3 \times 10^{-3}\text{eV}$ one still will be able to create a linear superposition of states $u_{250}(x, T) = a_{251} u_{251}(x, 0) + a_{253} u_{253}(x, 0) + a_{255} u_{255}(x, 0)$, which has a considerable “bump” near the center of the bundle. We would like to emphasize that direct microscopic simulations using Eq. (1) will need at least a thousand spatial discretization points that makes the problem currently computationally intractable.

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