Turning the BCS-BEC crossover into a phase transition by radiation.

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(Dated: May 20, 2015)

We show that the Bardeen-Cooper-Schrieffer state (BCS) and the Bose-Einstein condensation (BEC) sides of the BCS-BEC crossover can be rigorously distinguished from each other by the extrema of the spectrum of the fermionic excitations. Moreover, we demonstrate that this formal distinction is realized as a non-equilibrium phase transition under radio frequency radiation. The BEC phase remains translationally invariant, whereas the BCS phase transforms into the supersolid phase. For a two-dimensional system this effect occurs at arbitrary small amplitude of the radiation field.

PACS numbers: 67.85.-d; 67.85.Lm; 67.80.-s; 03.75.Kk

Introduction—The Bose-Einstein condensation (BEC) [1] and Bardeen-Cooper-Schrieffer state (BCS) [2] are two extreme scenarios for the formation of the superfluid state in fermionic systems where the only allowed gapless mode is the acoustic bosonic branch. In the BEC scenario, the fermions are first paired into compact two-particle complexes (molecules). These molecules experience Bose-Einstein condensation with the acoustic low energy spectrum due to the weak repulsion between molecules. In the BCS scenario, weakly coupled Cooper pairs are formed from states near the Fermi level so that the characteristic size for the pair correlation significantly exceeds the interparticle distance. Nevertheless, this weak coupling is sufficient to gap the fermionic excitation and leads to bosonic acoustic excitations as the oscillations of the order parameter. The physical effects occurring in between those two scenarios are referred to as BCS-BEC crossover.

The BCS-BES crossover is captured by the simplest Hamiltonian density [3]

\[ H = \psi_\sigma^* h(1) \psi_\sigma + b^* h(2)b + \left[ \frac{\lambda}{2} b^* \psi_{\sigma_1} \tau^y_{\sigma_1,\sigma_2} \psi_{\sigma_2} + h.c. \right], \]  

(1a)

where \( \sigma \) labels two (spin or pseudospin) states for the fermions described by Grassmann fields \( \psi_\sigma(\mathbf{r}), \psi_\sigma^*(\mathbf{r}) \) (summation over repeated indices is implied, and \( \tau^y \) is the standard Pauli matrix), and the bosonic fields \( b(\mathbf{r}), b^*(\mathbf{r}) \) describe the bound states of two fermions. The single specie energy part is described by (\( h = 1 \))

\[ h(1) \equiv (-i \nabla - q \mathbf{a})^2 / (2qm) + q \varphi - \delta_2, q \epsilon_b, \]  

(1b)

where the background vector \( \mathbf{a}(\mathbf{r}, t) \) and scalar potentials \( \varphi(\mathbf{r}, t) \) are introduced to highlight the continuity equation for the total particle density \( \psi_\sigma(\mathbf{r}) = \psi_\sigma^* \psi_\sigma + 2b^* b \).

The parameter \( \epsilon_b \) describes the energy of the bound state when \( \epsilon_b > 0 \) or the position of the resonance when \( \epsilon_b < 0 \). In models of pre-formed pairs in superconductors [4], \( \epsilon_b \) is a material dependent parameter. In experiments with cold atoms \( \epsilon_b \) is the directly tunable position of the Feshbach resonance [5, 6]. Thus, cold atom system provide a versatile platform for a detailed study of the BEC-BCS crossover.

In Eq. (1b), the constant \( \lambda \) controls the coupling of the bound state (molecules) with fermionic continuum. If \( \lambda \) is sufficiently small \( n^{2/D}/m \gg |\lambda| n^{1/2} \) (so-called narrow resonance regime), an analytic treatment of the problem is possible for any \( \epsilon_b \) and dimensionality \( D \) [7]. For large \( \lambda \) the crossover can be investigated only numerically [8].

Definition of the “critical field” of the crossover—The arguments below are independent of the width of the resonance. All numerical and analytical study of the ground state energy of the Hamiltonian (1a) at \( \varphi, a = 0 \) indicates that the ground state energy density \( E_{GS}(n, \epsilon_b) \) is an analytic function of its arguments, (hence the term crossover rather than transition). The usual argument is that regardless of the values of the parameters, the last term in Eq. (1a) leads to an anomalous average \( \langle \psi_\sigma \tau^y_{\sigma_1,\sigma_2} \psi_{\sigma_2} \rangle \propto (b) \propto e^{i\epsilon_b} \). Given that apparently no other symmetry breakings occur, there is no sharply defined critical field \( \epsilon^c_b(n) \) that separates the BEC and BCS regimes. Moreover, for all parameters the low energy excitations are described by superfluid hydrodynamics given by the Lagrangian

\[ \mathcal{L} = n \left[ \phi - \frac{\mathbf{v}^2}{2m} \right] - E_{GS}(n) + \gamma^*_\sigma \left[ i \partial_t - \epsilon(-i \nabla; n) \right] \gamma_\sigma, \]  

(2)

where \( \partial_t \equiv \partial_t + \mathbf{v} \cdot \nabla \) is the convective derivative, \( \phi \equiv \partial_t \varphi + \varphi \) and \( \mathbf{v} \equiv \nabla \varphi - a \) are the gauge invariant potential and velocities respectively, the fields \( n \) and \( \varphi \) are real, and \( \gamma_\sigma, \gamma^*_\sigma \) are the Grassmann fields describing the fermionic excitations (which for the problem of interest can be viewed as neutral BCS quasiparticles). This Lagrangian is an analytic function of variables, which apparently does not allow a definition of a critical field separating the two regimes. The first term in Lagrangian (2) is protected by the gauge and Galilean invariances and the second term, \( E_{GS}(n; \epsilon_b) \), is an analytic function of \( \epsilon_b \). This implies that the spectrum of the bosonic excitations (phonons) also must be analytic. However, the spectrum of the fermionic excitations \( \epsilon(k) \) experiences a reconstruction that allows for the definition of the critical
We will call the radius of the critical point (3a). For a finite perturbation of the ground state of the two-dimensional system it is possible to induce a spontaneous symmetry breaking that corresponds to the superfluid state via a weak quantum correction by itself is not observable, radiation above the threshold, $d > 0$, does not lead to any changes in the properties of the ground states of the system.

The situation changes qualitatively below the BEC-BEC transition, $\epsilon_b < \epsilon_c^\ast$. Indeed the minimal energy of the pair excitations is given by a fermion $f$ and a fermion $\gamma$ and (6) is the final answer. As this energy correction by itself is not observable, radiation above the threshold, $d > 0$, does not lead to any changes in the properties of the ground states of the system.

The correction $\delta E_{GS}^{(0)}$ is logarithmically divergent as $d \to 0$. This corresponds to a photon with energy just sufficient for the excitation of two excitations of the original problem (1). In the context of cold atom systems this would be given by a third hyperfine state. The radiation induces transitions between the third species and one of the fermions from Eq. (1), so that in terms of the low energy theory (2) it creates or annihilates two fermionic excitations,

$$H_{RF} = f^\ast \left( h^{(1)} + \Delta_f \right) f + \left[ F_\sigma(t) e^{-i\theta} f\gamma_{\sigma} + h.c. \right], \quad (4)$$

where $F(t)$ is proportional to the strength of the radiation field, and $\Delta_f > 0$ is the boundary of the spectrum of the third species. The functional form of the second term in Eq. (4) is protected by gauge invariance. Let us concentrate on the case of the monochromatic radiation $F(t) \propto e^{i\omega t}$, and introduce detuning as

$$d = \Delta(n, \epsilon_b) + \Delta_f - \omega. \quad (5)$$

If $d < 0$ the Hamiltonian (4) creates real fermion pairs and phonons and therefore leads to entropy growth (heating). For $d > 0$ real processes are not allowed (in fact, multi-photon real processes are also forbidden as the Hamiltonian (4) necessarily creates one $f$ particle per one photon), and the coupling (4) introduces a correction to the ground state energy density

$$\delta E_{GS}^{(0)} = \int \frac{d^2k}{(2\pi)^2} \mathcal{E}(k); \quad \mathcal{E}(k) = -\frac{F_\sigma F_{\sigma}^\ast}{\xi(k)}, \quad (6)$$

where $\xi(k) \equiv k^2/(2m) + \epsilon(k) - \Delta + d$ is the energy of the virtual state consisting of two excited fermions, and the meaning of the superscript (0) will become clear shortly.
a spontaneous breaking of translational symmetry to enable this process.

The resulting state has no currents and the variation of density $\delta n(r) \ll \langle n \rangle$ is periodic in space $\delta n(r + j_1 t_1 + j_2 t_2) = \delta n(r)$ (here $t_{1,2}$ are the primitive translation vectors). It can therefore be classified as a supersolid state. If the primitive vectors of the reciprocal lattice $b_{1,2}$ have the length of $k_F$, the excitation of the lowest state becomes allowed and the logarithmically divergent negative correction to the ground state is present. We will see that this correction can overcome the positive contribution to the ground state energy from the compressibility $(1/2)(\delta n)^2(\partial^2 E_{GS}/\partial n^2)_{F=0}$ thus making the supersolid state energetically favorable.

**Supersolid state and the phase diagram**—In the presence of the periodic density variation, the fermionic gap in Eq. (3b) also acquires a spatial variation, $\Delta \equiv (\partial \Delta/\partial n)_{n=0} \delta n$. The correction (6) changes due to the effect of the periodic potential produced by the supersolid:

$$\delta^{(n)} E_{GS} = - \sum_{b,\alpha} \int_{BZ} d^2k (2\pi)^2 \xi_{b,\alpha}(k); \quad \mathcal{E} = - \left| F_{b,\alpha}(\xi_{b,\alpha}(k)) \right|^2,$$

(7a)

where the quasimomentum integration is performed within the first Brillouin zone, $b$ is a vector of the reciprocal lattice, $\alpha$ labels the band for the $\gamma$ fermion in the periodic potential, described by Schrödinger equation for the Bloch functions, $u_{j,k}(r + t) = u_{j,k}(r)e^{ik\xi}$,

$$\left[ \beta (k_F^2 + \nabla^2)^2/4 + \tilde{\Delta}(r) \right] u_{\alpha,k}(r) = \tilde{\xi}_{\alpha}(k) u_{\alpha,k}(r).$$

(7b)

The energy of the two particle virtual state is $\xi_{b,\alpha}(k) \equiv d - \Lambda + (k + b)^2/(2m) + \tilde{\xi}_{\alpha}(k)$, and the matrix elements connecting excited states to the ground state are

$$F_{b,\alpha}(\xi_{b,\alpha}(k)) = F_{\sigma}/S_{uc} \int_{uc} d^2r e^{-i(k+b)\cdot r} u_{\alpha,k}(r).$$

(7c)

The integration is within the lattice unit cell of area $S_{uc}$, and Bloch functions are normalized as

$$\int_{uc} d^2r |u_{\alpha,k}(r)|^2 = S_{uc}.$$ 

(7d)

For $\tilde{\Delta} = 0$, equations (7) are nothing but the expression (6) folded into the first Brillouin zone, as all the other couplings (7c) vanish.

For small $\tilde{\Delta}$ the relevant part of the spectrum can be described in the almost free particle approximation. Consider triangular lattice

$$\tilde{\Delta}(r) = -\tilde{\Delta} \sum_{l=1}^6 \exp(ib_l \cdot r),$$

(8)

where the vectors $b_l$ are shown on Fig. 2 a).

On symmetry grounds only $A_1$ state, invariant under the symmetry group (see Fig. 2), can contribute to the matrix elements (7c) and

$$F_{\sigma}^{0,A_1}(\vec{k} = 0) = -\sqrt{6} \Delta \Lambda, \quad \tilde{\xi}_{A_1}(0) = -2\tilde{\Delta}.\quad (9)$$

The linear in $\tilde{\Delta}$ shift of the lowest energy level $\tilde{\xi}_{A_1}$ is the signature of the triangular symmetry, $D_6$; the shift makes this lattice the most energetically profitable in comparison with, e.g., square one.

The main contribution to the energy differences because the symmetry broken and the symmetric states comes from the lowest energy part of the spectrum. For the calculation with logarithmic accuracy, the partial contribution $\mathcal{E}$ can be approximately written as $\mathcal{E} \approx d - \Lambda - 2\Delta + k^2/(2m)$. It yields

$$\left[ \delta^{(n)} - \delta^{(0)} \right] E_{GS} = \frac{3\Delta^2 m}{\pi} \left[ - \frac{F_{\sigma}^2}{2\Lambda^2} Y(d - 2\Lambda) + y \right].$$

(10)

where the detuning from the lowest excitation energy is given by $d \equiv d - \Lambda$, and function $Y$ is defined as

$$Y(X) = \ln \left[ \frac{k_F^2}{(mX)} \right].$$

(11)

The last term in Eq. (10) is the compressibility contribution and the positive constant,

$$g \equiv (\pi/m)(\partial^2 E_{GS}/\partial n^2)_{F=0} (\partial \Delta/\partial n)^{-2},$$

(12)

is of the order of unity.

The correction given in Eq. (10) is the main result for the ground state energy at the lowest order in $|F|^2$. It shows that the broken symmetry supersolid state is always energetically profitable for any finite $F$. However the potential is apparently pathological, as $Y(X)$ diverges as $X \to 0$. This infinite growth is an artifact.
of the lowest in $F$ approximation, as the presence of the external field leads to the level repulsion. This level repulsion cuts the logarithm, and we turn to study of this effect.

For $|F| \ll \lambda$ it is sufficient to take into account only the two lowest energy states which couple to the radiation and their interaction with the reference state without fermions. Then, the partial energy function and their interaction with the reference state without the two lowest energy states which couple to the radiation in Eq. (10), where $\tilde{H}$ is defined as the Hamiltonian

$$\hat{H}_{eff} \approx \begin{pmatrix} d + \frac{k^2}{2m} & 0 & -\frac{F}{\lambda} \\ 0 & d - \Lambda - 2\tilde{\Delta} + \frac{k^2}{2m} & \frac{\sqrt{6}\tilde{\Delta}}{\lambda} \\ -\frac{\sqrt{6}\tilde{\Delta}}{\lambda} & \frac{\sqrt{6}\tilde{\Delta}}{\lambda} & 0 \end{pmatrix}.$$  \hspace{1cm} (13)

Straightforward calculation leads to the replacement

$$Y(\tilde{d} - 2\tilde{\Delta}) \rightarrow Y \left[ \sqrt{\tilde{d}(\tilde{d} - 2\tilde{\Delta})^2 + \frac{6\tilde{\Delta}^2|F|^2}{\Lambda^2}} \right]$$  \hspace{1cm} (10')

in Eq. (10), where $\tilde{d}(F) \equiv d - \Lambda + |F|^2/\Lambda$ has the meaning of the lowest energy of the two-fermionic excitations shifted by the RF field.

The resulting form of the energy profile (10), (10') is shown on Fig. 3. It shows two locally stable state characteristic of the first order phase transition. Direct inspection shows that the supersolid state becomes more energetically profitable when $|\tilde{d}(F)| \leq \tilde{d}_c(F)$ where the critical detuning is given by

$$Y \left( \frac{\sqrt{3}\tilde{d}_c(F)|F|^2}{2\Lambda^2} \right) = \frac{\Lambda^2 g}{|F|^2}.$$  \hspace{1cm} (14)

The resulting phase diagram is shown on Fig. 4.

In conclusion, we have noted the BCS-BES crossover is necessarily followed by the reconstruction of topology of the spectrum of the fermionic excitations and the critical field can be rigorously defined as the point of such change. We suggested an experimental scheme which transmutes this reconstruction of the excitation spectrum into a change in the symmetry of the ground state. For this scenario the supersolid state is predicted to form.

The actual process by which the supersolid state forms is apparently quite complex. The process is an inherently non-equilibrium, zero temperature and first order phase transition. Each of these features alone bring interesting facets to the issue of the phase transition kinetics. Therefore this transition could be an interesting arena for testing theories of phase transition kinetics.

We are grateful to O. Agam and L.I. Glazman for reading the manuscript and to A.D. Vlasov for participation in the initial stage of this project. This work was supported by Simons foundation.

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FIG. 3. The correction to the ground state energy as a function of the order parameter, for liquid a) and supersolid c) states. Though such energy profile is typical for the first order phase transitions, its functional form is different from the Landau type expansion.

FIG. 4. The proposed phase diagram at the fixed amplitude of the radiation field (main panel). The insets show the phase diagram at fixed position of the resonance $\epsilon_b$ in the BEC a) and BCS b) regions. The “hysteresis” region of the phase diagram depends on the preparation of the system and may correspond either to super-solid or the non-stationary normal phase heated by r.f.-radiation.
SUPPLEMENTAL MATERIAL: HYDRODYNAMICS IN THE NARROW RESONANCE LIMIT.

The purpose of this supplementary section is to obtain explicitly express the parameters of the hydrodynamic description [Eqs. (2) – (3) of the main text]. We restrict ourselves to the two-dimensional case, \( D = 2 \), in the narrow resonance regime,

\[
\eta \equiv \lambda \sqrt{n} \left( \frac{n}{m} \right)^{-1} \ll 1. \tag{S.1}
\]

Moreover, we will consider the position of the resonance \( \epsilon_b \) near the critical one \( \epsilon_c \) as discussed in the main text.

We begin with the Hamiltonian density (1) of the main text, setting all the gauge fields to zero.

\[
\hat{H} = b^\dagger \left( \frac{-\nabla^2}{4m} - \epsilon_b \right) b + c_{\sigma}^\dagger \left( \frac{-\nabla^2}{2m} \right) c_{\sigma} + \lambda \left[ b c_{\sigma_1}^\dagger \tau^y_{\sigma_1\sigma_2} c_{\sigma_2}^\dagger + h.c. \right]. \tag{S.2}
\]

As we are dealing with two-dimensional systems, all the observable quantities expressed via the bare parameters of the Hamiltonian contain logarithmic divergences, however, the relations between different observables are free of such divergences. To illustrate this point, we note that the quantity \( \epsilon_b \) is not the observable location of the resonance. We may calculate the physical resonance \( E_r \), by computing the correction to the energy of one \( b \) particle at zero momentum due to the excitations of two virtual fermions:

\[
\delta \Pi (\omega) = -\lambda^2 \int \frac{d^2k}{(2\pi)^2} \frac{1}{k_x^2 + m - \omega} = -\frac{m\lambda^2}{4\pi} \ln \left( \frac{\Lambda}{\omega} \right), \tag{S.3}
\]

where \( \Lambda \) is an unphysical high energy cutoff.

The physical location of the resonance is determined by the self-consistency equation

\[
E_r = -\epsilon_b - \frac{m\lambda^2}{4\pi} \ln \left( \frac{\Lambda}{|E_r|} \right), \tag{S.4}
\]

where \( \Lambda \) is some high-energy cut-off. The value of \( E_r \) is an observable position of the bound state at \( E_r < 0 \) and the position of the resonance at \( E_r > 0 \).

We proceed to calculate the properties of the ground in the in the saddle point approximation, which is valid in the narrow resonance regime. We take the spatially homogeneous ansatz

\[
b = \Delta/\lambda \in \mathbb{R}. \tag{S.5}
\]

and introduce the thermodynamic potential density so that

\[
E_{GS}(n) = \Omega(\mu) - \mu \partial_\mu \Omega(\mu), \tag{S.6}
\]
where $\mu(n)$ is found from

$$n = -\partial_\mu \Omega(\mu). \quad (S.7)$$

The thermodynamic potential $\Omega(\mu)$ is found as the ground state of the mean-field version of the Hamiltonian (S.2)

$$\hat{H} = - (2\mu + \varepsilon_b) \frac{\Delta^2}{\lambda^2} + c_\sigma^\dagger \left(-\nabla^2 - \mu\right) c_\sigma + \left[\frac{\Delta}{2} c_\sigma^\dagger \gamma^y \gamma^x c_\sigma + h.c.\right]. \quad (S.8)$$

After Bogoliubov rotation of the fermion operators in Eq. (S.8), we have their spectrum for small $k$ and small $\mu$ is

$$\epsilon(k) = \left[\frac{k^2}{2m} - \mu - \frac{k^2}{2m|\Delta|} + \frac{k^4}{8m^2|\Delta|}\right]^{1/2} \approx |\Delta| - \frac{k^2\mu}{2m|\Delta|} + \frac{k^4}{8m^2|\Delta|}. \quad (S.9)$$

Comparing (S.9) with Eq. (3b) of the main text we see that the critical point $\epsilon^c_b(n)$ is determined by $\mu = 0$. Since we are investigating the vicinity of the region around this critical point we can restrict ourselves small $\mu$ limit.

The thermodynamic potential at zero temperature is given by,

$$\Omega(\mu, \Delta) = (-\varepsilon_b - 2\mu) \frac{\Delta^2}{\lambda^2} + \int \frac{d^2k}{(2\pi)^2} \left\{ \frac{k^2}{2m} - \mu - \left[\left(\frac{k^2}{2m} - \mu\right)^2 + \Delta^2\right]^{1/2} \right\} \approx (-\varepsilon_b - 2\mu) \frac{\Delta^2}{\lambda^2} - \frac{m}{4\pi} \Delta^2 \ln \left(\frac{\sqrt{\varepsilon_b} \Delta}{\Delta}\right) + \mathcal{O}(\mu \Delta)$$

$$= (E_r - 2\mu) \frac{\Delta^2}{\lambda^2} - \frac{m}{4\pi} \Delta^2 \ln \left(\frac{\sqrt{\varepsilon_b} E_r}{\Delta}\right) + \mathcal{O}(\mu \Delta), \quad (S.10)$$

where in the last line the physical resonance $E_r$ from Eq. (S.4) is used to obtain the expression free of the logarithmic divergences.

Minimizing Eq. (S.10) with respect to $\Delta$ gives,

$$E_r - 2\mu = \frac{m\lambda^2}{4\pi} \ln \left(\frac{|E_r|}{\Delta}\right),$$

with the resulting expression for the fermionic gap

$$\Delta(\mu) = \Delta(0) \exp \left(\frac{8\pi\mu}{m\lambda^2}\right); \quad \Delta(0) = |E_r| \exp \left(-\frac{4\pi E_r}{m\lambda^2}\right) \quad (S.11)$$

and the thermodynamic potential

$$\Omega(\mu) = -\frac{m}{8\pi} \Delta^2(\mu); \quad \Omega(\mu) = -\frac{m}{8\pi} \Delta^2(\mu); \quad (S.12)$$

Varying $\mu$ and enforcing Eq. (S.7), we obtain

$$n = \frac{2\Delta^2(\mu)}{\lambda^2} \quad (S.13)$$

and the equation of states (S.6) as

$$E_{GS}(n) = \frac{mn\lambda^2}{16\pi} \ln \left(\frac{n\lambda^2}{2\varepsilon_b(0)}\right) \quad (S.14)$$

As noted above the critical detuning $\epsilon^c_b(n) = -E_r$ is defined by $\mu = 0$. Equations (S.11) and (S.13) give

$$\epsilon^c_b(n) = -\frac{m\lambda^2}{4\pi} \ln \left(\frac{\sqrt{\varepsilon_b} E_r(n)}{\lambda\sqrt{n}}\right)$$

which with the logarithmic accuracy yields.

$$\epsilon^c_b(n) = -\frac{m\lambda^2}{4\pi} \ln \left(\frac{2^{1/2}}{\pi} \eta\right) \quad (S.15)$$

The values of the remaining parameters entering into Eq. (3b), thus are [see Eq. (S.9)]

$$\Delta = \frac{\lambda\sqrt{n}}{\sqrt{2}}, \quad \alpha = \frac{1}{4m\Delta}, \quad \beta = \frac{1}{8m^2\Delta} \quad (S.16).$$