Molecular Kondo Resonance in Atomic Fermi Gases

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The usual Kondo effect is associated with the formation of a many-body ground state that contains a quantum-mechanical entanglement between a (localized) fermion and the free fermions. We show, however, that also a bosonic form of the Kondo effect can occur in degenerate atomic Fermi gases near a Feshbach resonance, if the energy of the diatomic molecular level associated with the Feshbach resonance approaches twice the Fermi energy of the atoms.

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Introduction.—The Kondo effect is an intricate many-body phenomenon that was originally put forward to explain the anomalous resistance minimum of metals contaminated with magnetic impurities. Today the Kondo effect is known to be also responsible for the existence of heavy-fermion materials [1], and is speculated to play an important role in the physics of high-temperature superconductors [2]. Moreover, a particularly clear manifestation of this effect occurs in semiconductor quantum dots [3,4]. In all these examples the Kondo effect is associated with the formation of a many-body ground state that contains a quantum-mechanical entanglement between a (localized) fermion and the free fermions. Here we show that a new version of the Kondo effect can occur in the degenerate atomic Fermi gases with a so-called Feshbach resonance that have recently been created [5–8]. In contrast to the usual fermionic version, the many-body ground state of the atomic gas shows coherence between bosons, in fact bosonic molecules, and the free fermions in the gas. We show that this bosonic Kondo effect occurs if the energy of the molecule is somewhat larger than twice the Fermi energy of the atoms. We also discuss how it can be observed experimentally.

To be concrete we consider a homogeneus degenerate Fermi gas of ^{3}Li or ^{40}K atoms near a so-called Feshbach resonance [8–11]. A Feshbach resonance in the scattering amplitude of two alkali atoms arises when the energy of the two colliding atoms is close to the energy of a diatomic molecular state that is coupled to the incoming atoms. Since the coupling is provided by the hyperfine interaction between the electron and nuclear spins of the atoms, the magnetic moment of the molecule is not equal to twice the atomic magnetic moment. As a result, the Zeeman interaction leads to an energy difference between the incoming atoms and the molecule, and therefore to an effective interaction strength between the atoms, that is tunable by means of an external magnetic field. The usefulness of these Feshbach resonances for degenerate atomic gases was first pointed out theoretically [12,13] and then confirmed experimentally in a Bose-Einstein condensate of ^{23}Na atoms [14]. Feshbach resonances appear to be particularly useful for ultracold Fermi gases because of the possibility to achieve a Bose-Einstein condensation of Cooper pairs at experimentally accessible temperatures in this way [15–17]. For our purposes it is most important to realize that, due to the nearby location of a molecular state, the atomic gas can develop coherence between atoms and molecules. In a degenerate Bose gas the atom-molecule coherence has last year been demonstrated experimentally by Donley *et al.* [18]. It is the purpose of this Letter to point out that in the case of a degenerate Fermi gas it leads to Kondo physics.

Atom-molecule model.—In a dilute gas at low temperature only s-wave scattering is important. In a gas of fermionic particles, resonant interaction effects can therefore only be observed if we consider a mixture of two hyperfine states, denoted by $|\uparrow\rangle$ and $|\downarrow\rangle$. Close to resonance the gas is then described by an effective atom-molecule action [19]. In this action atoms in different hyperfine states are coupled to molecular bosons with twice the atomic mass m. In the absence of the coupling, the energy of the molecules relative to the two-atom continuum threshold is equal to the magnetic-field dependent detuning energy $\delta(B)$. The coupling terms describe processes in which two fermionic atoms form one bosonic molecule or the bosonic molecule breaks up into two fermionic atoms. The effective coupling strength g corresponds physically to the bare atom-molecule coupling dressed with ladder diagrams to take into account all two-body processes. According to this renormalization procedure, the parameters g and $\delta(B)$ of the effective atom-molecule theory can be expressed solely in terms of the experimentally known location of the Feshbach resonance B_0, its width ΔB, the associated magnetic moment difference $\Delta\mu_{\mathrm{mag}}$, and the nonresonant scattering length a_{bg}. In detail we have $g = \hbar\sqrt{4\pi a_{\mathrm{bg}}\,\Delta B\,\Delta\mu_{\mathrm{mag}}/m}$ and $\delta(B) = \Delta\mu_{\mathrm{mag}}(B - B_0)$ [19].

We consider here only the case of an equal number of atoms in every hyperfine state, and hence there is only one chemical potential μ. To avoid Bose-Einstein

condensation of the molecules, we consider a positive detuning that is larger than twice the chemical potential μ of the atoms. In this case no stable molecular state exists, and the molecule always has a short lifetime because it can decay into two free atoms. This finite lifetime is incorporated by the imaginary part of the molecular self-energy as we show next.

Spectral weight function.—Because we are mostly interested in the density of states of the molecules, we focus here on the spectral properties of the molecular Green's function and, in particular, how they are affected by the presence of the Fermi sea of atoms. According to quantum many-body theory, the molecular density of states is related to the spectral function $\rho_{\mathrm{m}}(\mathbf{q}, \omega)$, which is found from the retarded Green's function or propagator by means of $\rho_{\mathrm{m}}(\mathbf{q}, \omega) = -\mathrm{Im}[G_{\mathrm{m}}^{(+)}(\mathbf{q}, \omega)]/\pi\hbar$ and obeys the sum rule $\int_{-\infty}^{\infty} d(\hbar\omega)\, \rho_{\mathrm{m}}(\mathbf{q}, \omega) = 1$. The exact molecular retarded propagator is $G_{\mathrm{m}}^{(+)}(\mathbf{q}, \omega) = \hbar/[\hbar\omega + 2\mu - \delta(B) - \epsilon_{\mathbf{q}}/2 - \hbar\Sigma_{\mathrm{m}}^{(+)}(\mathbf{q}, \omega)]$, where $\epsilon_{\mathbf{q}} = \hbar^2\mathbf{q}^2/2m$ and $\hbar\Sigma_{\mathrm{m}}^{(+)}(\mathbf{q}, \omega)$ is the exact retarded self-energy. The problem thus reduces to the evaluation of the self-energy of the molecule. In the presence of a degenerate Fermi gas at temperatures far below the Fermi temperature, a zero-temperature approximation to the Fermi gas can be adopted. For the low-energy Kondo physics of interest to us, the energy dependence of the coupling constant g can be neglected as well. Moreover, we have checked that, within the weak-coupling limit of the Kondo effect that we only consider here, it is appropriate to consider the fermionic propagators as free and neglect mean-field effects due to interactions between the fermions in different spin states. In the ladder approximation the self-energy is determined by a Feynman diagram that physically describes the process of a molecule decaying into two atoms and subsequently recombining into a molecule again. Summing over all ladder diagrams ultimately yields

$$\hbar\Sigma_{\mathrm{m}}^{(+)}(\mathbf{q}, \omega) = -\eta i\sqrt{\hbar\omega + 2\mu - \frac{\epsilon_{\mathbf{q}}}{2}} + 2\eta\frac{\sqrt{2\mu}}{\pi} + \eta\frac{\hbar\omega}{\pi\sqrt{2\epsilon_{\mathbf{q}}}}\ln\left[\frac{\hbar\omega - \epsilon_{\mathbf{q}} + 2\sqrt{\mu\epsilon_{\mathbf{q}}}}{\hbar\omega - \epsilon_{\mathbf{q}} - 2\sqrt{\mu\epsilon_{\mathbf{q}}}}\right] + \frac{\eta}{\pi}\sqrt{\hbar\omega + 2\mu - \frac{\epsilon_{\mathbf{q}}}{2}}\left[\ln\frac{\sqrt{\hbar\omega + 2\mu - \frac{\epsilon_{\mathbf{q}}}{2}} - (\sqrt{2\mu} + \sqrt{\frac{\epsilon_{\mathbf{q}}}{2}})}{\sqrt{\hbar\omega + 2\mu - \frac{\epsilon_{\mathbf{q}}}{2}} + (\sqrt{2\mu} + \sqrt{\frac{\epsilon_{\mathbf{q}}}{2}})} + \ln\frac{\sqrt{\hbar\omega + 2\mu - \frac{\epsilon_{\mathbf{q}}}{2}} - (\sqrt{2\mu} - \sqrt{\frac{\epsilon_{\mathbf{q}}}{2}})}{\sqrt{\hbar\omega + 2\mu - \frac{\epsilon_{\mathbf{q}}}{2}} + (\sqrt{2\mu} - \sqrt{\frac{\epsilon_{\mathbf{q}}}{2}})}\right], \quad (1)$$

where $\eta = g^2m^{3/2}/4\pi\hbar^3$.

The bosonic spectral function for two different values of the detuning $\delta(B)$ is shown in the insets of Fig. 1. In the upper inset the detuning is much larger than the Fermi energy, or more precisely $\delta \gg \eta\sqrt{2\mu}$. In that case there is essentially no Kondo effect, and the spectral function shows just a single broad peak centered around the detuning. This is the expected situation for a single molecular state with a finite lifetime. In the lower inset the detuning is much closer to twice the Fermi energy and, apart from the broad feature around the detuning, the spectral density now also shows slightly above and below zero frequency two sharp peaks. This is the Kondo effect. Physically these two sharp peaks are a pure many-body effect due to a logarithmic singularity in the self-energy that is induced by the Fermi surface. They signal the formation of a molecular resonance that contains a quantum-mechanical entanglement between the bosonic molecule and the free fermions. The situation is reminiscent of the Anderson model for a quantum dot, with a localized electron level located just below the Fermi energy of the leads. In that model the on site Coulomb repulsion on the quantum dot removes the symmetry between scattering to and from the dot and leads to a logarithmic singularity in the self-energy. In our case no Coulomb blockade is required and the formation of the Kondo resonance is the result of the fact that the molecule consists of two atoms. If a molecule breaks apart, it adds two particles to the Fermi sea. As a result our Hamiltonian is not quadratic in creation and annihilation operators and contains much more physics than the Anderson model without on site Coulomb interaction, i.e., the Fano-Anderson model which has no Kondo resonance. The role of the localized fermion is now played by the bosonic molecular state above the two-particle Fermi surface, and the Kondo resonance appears slightly above twice the Fermi energy because otherwise the equilibrium situation would be a Bose-Einstein condensate of molecules.

In the weak-coupling limit the resonant molecular state with zero momentum has exactly the same form as the wave function underlying the Kondo effect in the Anderson model. In the latter case we have [20]

$$|\Psi_{\mathrm{K},\sigma}\rangle = \sqrt{Z}f_\sigma^\dagger|\Phi_{\mathrm{F}}\rangle + \sum_{|\mathbf{k}|>k_{\mathrm{F}}} u_{\mathbf{k}}c_{\mathbf{k},\sigma}^\dagger|\Phi_{\mathrm{F}}\rangle + \sum_{|\mathbf{k}|<k_{\mathrm{F}}} v_{\mathbf{k}}f_\sigma^\dagger f_{-\sigma}^\dagger c_{\mathbf{k},-\sigma}|\Phi_{\mathrm{F}}\rangle, \quad (2)$$

where $|\Phi_{\mathrm{F}}\rangle$ is the filled Fermi sphere, k_{F} is the Fermi momentum, and $c_{\mathbf{k},\sigma}^\dagger$ and $f_\sigma^\dagger$ are the creation operators for the conduction electrons and the electrons on the dot, respectively. The only difference with the Anderson model is that in our situation fermions are created above and below the Fermi sea in pairs. Hence we have

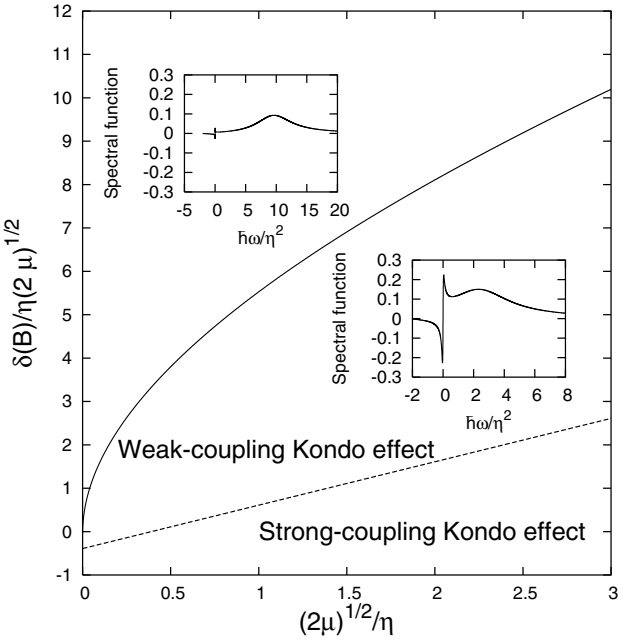

FIG. 1. The phase diagram for the bosonic Kondo effect. Above the solid line the Kondo effect is for all practical purposes invisible, whereas below this line there appears a Kondo resonance in the molecular spectral function. The dashed line found from $k_B T_K = 2\mu$ marks the crossover to the strong-coupling regime. In the insets we show the zero-momentum molecular spectral function in units of $1/\eta^2$ and as a function of frequency, for two different values of the parameters $\delta(B)/\eta\sqrt{2\mu}$ and $\sqrt{2\mu}/\eta$. In the upper inset $\delta(B)/\eta\sqrt{2\mu} = 12/\sqrt{2}$ and $\sqrt{2\mu}/\eta = \sqrt{2}$. In the lower inset $\delta(B)/\eta\sqrt{2\mu} = 5/\sqrt{2}$ and $\sqrt{2\mu}/\eta = \sqrt{2}$.

$$|\Psi_K\rangle = \sqrt{Z} b_0^\dagger |\Phi_F\rangle + \sum_{|\mathbf{k}|>k_F} u_\mathbf{k} c_{\mathbf{k},\uparrow}^\dagger c_{-\mathbf{k},\downarrow}^\dagger |\Phi_F\rangle + \sum_{|\mathbf{k}|<k_F} v_\mathbf{k} b_0^\dagger b_0^\dagger c_{\mathbf{k},\uparrow} c_{-\mathbf{k},\downarrow} |\Phi_F\rangle, \quad (3)$$

where $b_0^\dagger$ and $c_{\mathbf{k},\sigma}^\dagger$ are our bosonic and fermionic creation operators. In the two-atom limit, where the Fermi sea $|\Phi_F\rangle$ becomes the vacuum state and no Kondo effect is present, the hole amplitude $v_\mathbf{k}$ vanishes and the molecular wave function has only contributions from the bare molecular state, with amplitude $\sqrt{Z}$, and from the two-atom continuum, with particle amplitudes $u_\mathbf{k}$. This wave function indeed describes exactly the dressed molecule of the Feshbach resonance that exists for negative detuning. When the Fermi surface is present, pairs of fermionic atoms with opposite spin tunnel back and forth from the Fermi sea into the molecular state. The coherent addition of many of such events produces the Kondo effect. It is important to realize that because the molecules are bosons, the negative peak below the Fermi energy and the positive peak above the Fermi energy are both physically associated with the same molecular state. The presence of the negative peak just indicates that molecular states are populated even at zero temperature.

Kondo temperature.—The energy of the Kondo resonance is equal to $k_B T_K$, where T_K is the so-called Kondo temperature. This temperature plays an important role because in the Kondo regime it is possible to express all the temperature effects as universal functions of T/T_K. Moreover, it is the temperature to which the Fermi gas needs to be cooled experimentally to observe the Kondo effect. In the weak-coupling limit it is given by $T_K = \frac{8\mu}{e^2 k_B} e^{(\pi/2)(\sqrt{2\mu}/\eta)} e^{-(\pi/2)[\delta(B)/\eta\sqrt{2\mu}]}$. This nonperturbative result is, apart from the prefactor, identical to the Kondo temperature of the Anderson model in the weak-coupling limit that is given by $T_K \propto (\mu/k_B) e^{-\delta/g^2 N(0)}$, where δ is the energy difference between the state on the quantum dot and the Fermi level, g is the hopping parameter between the conduction electrons and the dot, and $N(0)$ is the density of states at the Fermi level.

The Kondo temperature makes it possible to classify two different limits. When $k_B T_K \ll 2\mu$, the system is in the weak-coupling regime. Otherwise we are dealing with a strong-coupling situation. The dashed line in the phase diagram shown in Fig. 1 marks this separation in the parameter space. The theory presented here allows for a full description of the weak-coupling limit, while for a strong-coupling treatment an improved approximation in the calculation of the molecular self-energy is needed. In particular, it will be necessary to consider the resonant interactions between the fermions, which lead to the creation of particle-hole pairs in the Fermi sea.

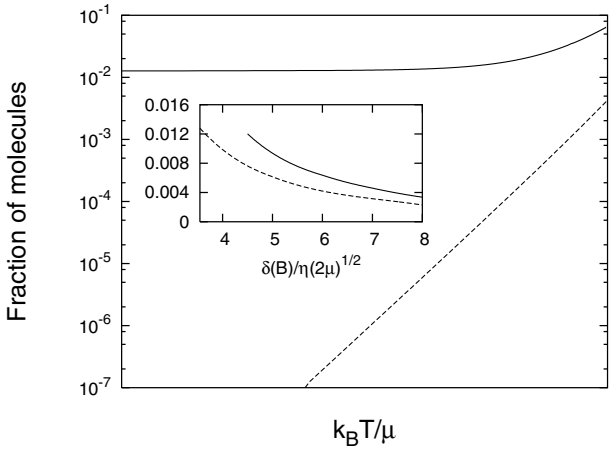

FIG. 2. Fraction of molecules in the gas as a function of temperature. The solid line shows the result for the parameter $\delta(B)/\eta\sqrt{2\mu} = 5/\sqrt{2}$ and $\sqrt{2\mu}/\eta = \sqrt{2}$. The dashed line shows the maximum number of molecules that can be achieved without many-body effects. In the inset the fraction of molecules at zero temperature is plotted as a function of the detuning for two different values of the chemical potential. The solid and the dashed lines show the result when $\sqrt{2\mu}/\eta = 2$ and when $\sqrt{2\mu}/\eta = \sqrt{2}$, respectively.

Experimental signature.—In order to observe the Kondo effect, its associated resonance must contain sufficient spectral weight. Using that the integrated weight of the Kondo peaks in the spectral function is proportional to $k_B T_K/\eta\sqrt{2\mu}$, the solid line in Fig. 1 gives a quantitative estimate of the lower limit for the visibility of the effect. Using typical parameters of ^{6}Li and ^{40}K, we have checked that the Kondo regime is indeed experimentally accessible. The direct experimental measurement of this Kondo effect can be accomplished by looking at the enhancement in the density of molecules even for relatively large detuning. For example, the recently developed spectroscopic method for sensitive detection of molecules in cold atomic gases could be used for this purpose [21]. Note that this method indeed measures the density of (bare) molecules because the different spin state of the closed channel of the Feshbach problem provides a selection rule for the optical transition used in this experiment. Also, the projection technique introduced by Regal *et al.* [22] is a method to determine the (bare) molecule content of the gas.

The influence of the Kondo effect on the total number of molecules in the gas can be easily calculated. At temperatures $T \ll \mu/k_B$, it is consistent to calculate the total density of the bosonic molecules in the gas by multiplying the zero-temperature molecular spectral function with the Bose distribution function $N(x) = [e^x - 1]^{-1}$ and integrating over all momenta and frequencies, i.e., $n_B(T) = \int_{-\infty}^{+\infty} d(\hbar\omega) \int [d\mathbf{q}/(2\pi)^3] \rho_m(\mathbf{q}, \omega) N(\hbar\omega/k_B T)$. At zero temperature and without many-body effects, the number of molecules is exactly zero because the detuning is larger than the Fermi energy. When the Kondo resonance is included, even at zero temperature a nonzero number of molecules is obtained. The inset of Fig. 2 shows the molecular fraction in the gas at zero temperature for different values of the detuning. The thermal effects on the number of molecules are also shown in Fig. 2. Notice the enormous enhancement in the number of molecules due to the Kondo effect. It is also interesting to observe that without the many-body effects the maximum number of molecules goes to zero as T^3, whereas with the Kondo effect it saturates to a nonzero constant only as T^2. Since our calculations are valid within the weak-coupling limit, results are shown only for this regime.

It is important to realize that the Kondo temperature found above is always larger than the critical temperature of the Bose-Einstein condensation of Cooper pairs and, therefore, more easy to obtain experimentally. In the weak-coupling limit this critical temperature is known in terms of the s-wave scattering length $a(B)$ [15] as $T_{BCS} = (8e^{\gamma-2}\mu/\pi k_B) e^{\pi/2k_F a(B)}$, where γ is Euler's constant. Using the fact that the resonant part of this scattering length is given by $-g^2 m/4\pi\hbar^2\delta(B)$ allows us to express the Kondo temperature in terms of the BCS critical temperature as $T_K = \pi e^{(\pi/2)(\sqrt{2\mu}/\eta)-\gamma} T_{BCS}$, which is indeed always larger than the BCS critical temperature. Nevertheless, it must be pointed out that since only the parameters of the resonant part of the interaction play a role for the Kondo effect, T_K is physically quite distinct from T_{BCS}. In particular, we can have the situation of a positive total scattering length with no Cooper pairing at any temperature but with the Kondo effect still present.

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