Semiclassical polaron dynamics of impurities in ultracold gases

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(Dated: May 22, 2014)

We present a semiclassical treatment of a fermionic impurity coupled to Bogolyubov modes of a BEC. In the lowest order approximation we find a full solution of an initial value problem, which turns out to behave differently in the sub- and supersonic regimes. While in the former case no impurity deceleration is observed, in the latter case non-Markovian dissipation effects kick in resulting in slowing down of the fermion. Although this scenario is compatible with the one offered by an elementary field theoretical picture at weak coupling, the details of the dynamics turn out to be completely different. Fluctuation effects can be taken into account by expanding around the classical path, which leads to a natural cutoff scale for the momentum integrals of the order of the inverse polaron radius. As an application we calculate the drag force which is exerted by the BEC on the impurity moving with constant velocity $v$. Contrary to the perturbative result, according to which the drag force is $\sim v^2$, it turns out to be proportional to $1/v^2$ in the semiclassical regime.

PACS numbers: 03.75.Mn, 71.38.Fp, 67.85.Pq, 78.20.Bh

Interacting ultracold gases offer unique opportunities for the modeling of realistic quantum systems \cite{1}. During the recent years it not only became possible to study such exotic phenomena as BEC-BCS crossover, but also the modeling of systems inspired by the fractional quantum Hall effect might soon be within reach \cite{2–4}. One of very interesting and old condensed matter physics phenomena, which shows exciting physics on the one hand and on the other hand might immensely profit from parameter adjustability offered by ultracold gas systems is the polaron problem \cite{5}. In its simplest realization it describes electrons in a semiconductor which interact with phonons of the background lattice. The most important feature of the model is a fundamental difference in the properties of the system for weak and strong coupling between the fermionic and bosonic subsystem.

It turns out that polaron-like models can very effectively be simulated by fermionic impurity atoms immersed into a BEC \cite{6, 7}. Alternatively one can couple them to a continuum of bosonic excitations of some other fermionic species \cite{8}, or even use bosonic impurities of the species different from the one constituting the BEC bath. A direct mapping of most of the results from the vintage literature is, however, not possible for a number of reasons. First of all, the spectrum of bosonic excitations is usually profoundly different from those in a semiconductor. The second distinction is the coupling mechanism between the subsystems. Some less important details such as the presence and nature of cut-off parameters might drastically alter the properties of a given system as well. But the most important difference is at the same time an enormous advantage – it is the adjustability of parameters, which is far superior to that in solid state realizations. This feature makes it possible to advance into new and as yet unexplored parameter regions. One such situation is the semiclassical limit, in which the impurity can be considered to be an almost classical particle. Not only is this particular parameter constellation so far poorly understood, it also allows for a physically intuitive characterization of dynamics in super- and subsonic velocity regimes that have mostly been investigated using involved numerical methods in similar systems before \cite{9, 10}.

We consider a single fermionic impurity interacting with a gas of bosons with masses $m$ (we use polaronic units, where the mass of the impurity $m_I$ as well as the healing length of the BEC $\xi$ and the reduced Planck constant $\hbar$ are set to unity, throughout the Letter). The Hamiltonian reads

$$H = \frac{p^2}{2} + \sum_k \epsilon_k a_k^\dagger a_k + \frac{1}{2} \sum_{k,k',q} V_{BB}(q) a_{k'-q}^\dagger a_{k+q} a_k a_{k'} + \sum_{k',q} V_{IB}(q) \rho(q) a_{k'-q}^\dagger a_{k'},$$

(1)

where $a_k^\dagger$ and $a_k$ are the creation and annihilation operators for a boson with momentum $k$, $p$ is the momentum operator of the impurity, $V_{BB}$ and $V_{IB}$ are general boson-boson and impurity-boson interaction potentials, and the dispersion of the bosons is given by

$$\epsilon_k = \frac{k^2}{2m} - \mu.$$ 

(2)

$\mu$ is the chemical potential. The momentum space density of a point particle is related to its position operator $x$ via

$$\rho(q) = \int d^3y \delta^3(y-x)e^{iq\cdot y}.$$ 

(3)

Since we assume a dilute homogeneous gas, we perform the Bogoliubov approximation by replacing the zero
mode operators $a_0$, $a_0^\dagger$ by $c$-numbers [11]. We furthermore use contact pseudo-potentials for the interactions $V_{BB}(q) = g_{BB}$, $V_{IB}(q) = g_{IB}$, where the constants $g_{BB}$ and $g_{IB}$ are related to the $s$-wave scattering lengths of the true potentials via the Lippman-Schwinger equation. We then obtain a variant of the Fröhlich Hamiltonian [7, 12]

$$H = \frac{p^2}{2} + \sum_k \epsilon_k b_k^\dagger b_k + \sum_k V_k e^{ikx} \left(b_k + b_k^\dagger\right). \quad (4)$$

For reasons that will become clear below, we restrict the dispersion relation of the Bogoliubov quasiparticles $\epsilon_k$ and the interaction structure $V_k$ to the expressions valid for momenta that are smaller than the healing length in the BEC. Therefore, we have

$$\epsilon_k = ck, \quad V_k = \sqrt{\alpha k}, \quad (5)$$

where $c = 1/(\sqrt{2m})$ is the sound velocity in the BEC and the dimensionless coupling constant $\alpha$ can be related to the density $n$ of the bosonic gas and the impurity-boson interaction constant via $\alpha = n g_{IB}^2 / \sqrt{2}$.

Using the standard procedures, we can now integrate out the environmental (BEC) degrees of freedom, see for example [13]. A requirement for a semiclassical treatment is that the average wavelength of the impurity be small compared to a typical length scale of the system [14]. The latter is given by the healing length $\xi$, since it is the typical length on which the effective potential seen by the particle varies. The wave length of the impurity particle is in a first approximation given by $\lambda = \hbar / (vm_1)$, where $v$ is its velocity. Since the healing length is proportional to $\hbar / (\alpha m)$, we see that a large impurity mass compared to the masses of the bosonic particles justifies a semiclassical treatment. Moreover, we will mostly be interested in impurity velocities $v \geq c$, so that, for instance, an $^{85}$Rb impurity in a gas of $^{23}$Na should well be described by this theory. For the case in which $m_1 < m$ however, we still expect this approximation to be valid for very fast impurities with $v \geq mc/m_1$. Alternatively, in the strong coupling regime, where $\alpha \geq 1$ the self-trapping effects are expected to restrict the extent of the polaron wave function to a region smaller than the healing length of the BEC [7], or equivalently, the strong coupling leads to the generation of a large effective impurity mass. Apart from these effects, the dynamical aspects of the physics can then still be captured by the classical equations of motion, provided one works with the effective quantities.

In order to preserve the convergence of the integrals within the employed approximation, it is necessary to employ a cutoff scheme [15]. For reasons which become clear below we use a Gaussian $e^{-k^2/k_c^2}$ where $k_c$ is proportional to the inverse of the size of the polaron particle. The resulting EOM in three dimensions is then given by

$$\ddot{x}(t) = -\int_0^t du \gamma_{ij}(t-u)x_j(u) \quad (6)$$

with a generalized damping kernel

$$\gamma_{ij}(s, r) = \delta_{ij} \frac{\alpha k_c^3}{16\pi \sqrt{2} c s^3} e^{-\frac{1}{2} k_c^2 c s^2} \left\{ (e^{cs k_c^2 r} + 1) \left( c^2 s^2 k_c^2 r + k_c^2 r^3 \right) - (e^{cs k_c^2 r} - 1) \left( 1 + k_c^2 r^2 \right) \right\} + \frac{\gamma_j}{2r} \left\{ (e^{cs k_c^2 r} - 1) \left( 3cs \left( 4 + 2k_c^2 r^2 + k_c^2 r^4 \right) - k_c^2 r^2 c s^3 \right) - (e^{cs k_c^2 r} + 1) \left( 3k_c^2 c^2 s^2 r^2 \left( 2 + k_c^2 r^2 \right) + k_c^4 r^5 \right) \right\}, \quad (7)$$

where $r = x(t) - x(u)$. The dependence of the rhs of Eq. (6) on $r$ is a major structural difference to the case of linear coupling to the environment as in the Caldeira-Leggett model [10]. This results in a dissipation dynamics which is completely different. The influence of such a non-Markovian dissipation scenario is weak for short time scales and much of the dynamics can be described by an effective Caldeira-Leggett model. However, the deviations are drastic for intermediate and long times. In this case the solution of the initial value problem can only be found numerically [17]. We solve Eq. (6) for the initial value $x(0) = 0$ and $\dot{x}(0) = v_0$. As long as $v_0 < c$ (subsonic initial velocity) the difference to a solution in which $r = 0$ is set on the rhs of Eq. (7) throughout is minimal, see Fig. 1. On the contrary, in the supersonic case $v_0 > c$ the non-Markovian dissipation leads to drastic discrepancies. In the transient regime we observe distinct damped oscillations which can be connected with the appealing physical picture emerging in the elementary self-consistent harmonic approximation [3], according to which the polaron cloud is modeled as an additional mass on a spring attached to the impurity. An important point is the fact that both approximations cover the nonperturbative regime.

Despite its efficiency the numerical procedure is not able to produce reliable results for the long-time asymptotics of the particle. In order to obtain it one has to rely on simplifications of the basic equation [3]. As we have
shown above, the dependence of the rhs on the details of the particle trajectory at previous times via \( r \) is an obstacle. However, if we are interested in the long-time limit, we can neglect fast fluctuations of the particle velocity, as seen in the numerical simulations. Thus we can expand \( r(t, u) = v(t)(t - u) + \ldots \) and require \( v(t) \) to be self-consistently calculated. For the long-time asymptotics one then obtains the following EOM for the component of the displacement along the initial velocity \( v_0 \):

\[
\lim_{t \to \infty} \tilde{x}(t) = \frac{\alpha}{8\pi} \frac{c k_0^4 (c - \dot{x}(t) - |c - \dot{x}_i(t)|)}{(c - \dot{x}(t))\dot{x}(t)^2}
\]

It is important to note that in this effective equation for the long time behaviour of the particle coordinate, memory effects have not been neglected, but incorporated into the \( t \to \infty \) limit. The rhs is zero for \( v(t) < c \) and \( \propto v(t)^{-2} \) otherwise. This means that the solution to the initial value problem \( x(0) = 0, \dot{x}(0) = v_0 \) with Eq. (8) is

\[
x(t) = \begin{cases} 
  v_0 t \\
  \frac{c}{\alpha k_0^2} \left( v_0^4 - 3v_0^3 - \frac{3\alpha c k_0^2}{8\pi} t \right)^{4/3} 
\end{cases}
\]

otherwise

(9)

Especially the deceleration process of an initially supersonic impurity shows up interesting features. As long as \( v(t) > c \) the particle slows down and just above the threshold \( c \) the velocity decrease follows a power law \( \propto t^{-1} \) with exponent \( 1/3 \), see Fig. 2. After \( v \) drops below \( c \) it does not change any more. From the qualitative point of view this behaviour is to be expected, being a manifestation of superfluidity in the BEC. However, the change of velocity is smooth in previous perturbative studies \[18\] as opposed to our result, in which the time derivative of \( v \) shows a jump. Furthermore, the emergence of the critical velocity \( c \) is clearly a consequence of the nonlinear coupling: The long time behaviour of the corresponding EOM in which \( r = 0 \) is just that of a free particle, independent of its velocity, as can easily be shown using Laplace transform techniques.

As we have already mentioned above, \( k_0^{-1} \) can be connected to the conventional polaron radius. To see this, we note that when we take into account quadratic fluctuations around the classical path \( x(t) \) (see e.g. \([19, 20]\)), Eq. (9) becomes a generalized Langevin equation in which a noise term \( \xi(t) \) has to be added to the rhs. \( \xi(t) \) is a Gaussian stochastic process with average \( \langle \xi(t) \rangle = 0 \) and state-dependent autocorrelation function

\[
\langle \xi_i(t) \xi_j(u) \rangle = \text{Re} \sum_k k_{ik} k_{jk} \frac{\alpha k}{2} G_k(t - u, \beta) e^{ikr},
\]

where \( G_k(t - u, \beta) \) is the real-time propagator for a boson of momentum \( k \) at inverse temperature \( \beta \). As required by the fluctuation-dissipation theorem, in the limit \( \beta \to \infty \), the rhs reduces to \( \gamma(t - u, r)/2 \). When taking averages over realizations of the noise of the full Langevin equation, \( \xi_i(t) \) no longer explicitly occurs on the rhs of the EOM, but we encounter averages of the form

\[
\langle e^{ikr} \rangle = e^{ik(r - (r') - (r')^2)/6},
\]

where we assumed that for every \( t, u \), the random variable \( r = x(t) - x(u) \) can be appropriately approximated by having Gaussian statistics. Therefore, from Eq. (11),
FIG. 3: Asymptotic behavior of the drag force for \( t \to \infty \) as a function of the drag velocity \( v_0 \). In the subsonic regime, it is zero as expected. It jumps to finite value just above \( v_0 = c \), subsequently decaying like \( 1/v_0^2 \). Inset: drag force as a function of time for drag velocities \( v_0 = 0.7c \) (solid line), \( v_0 = c \) (dashed line), \( v_0 = 1.2c \) (dashed-dotted line) and \( v_0 = 2c \) (dotted line).

we see that a natural cutoff for the \( k \)-sums is provided by the mean square of \( r \). In a stationary situation, we would expect that \( \langle r^2 \rangle \rightarrow \langle r^2 \rangle \rightarrow \langle x(t)x(u) \rangle \rightarrow \langle x(t)\rangle \langle x(u) \rangle \), which for \( u \to t \) can be considered to be a measure for the squared polaron radius \( r_{\text{pol}} \). Therefore, in this approximation

\[
 k_c \approx \frac{6}{r_{\text{pol}}^2}.
\]

For a coupling constant \( \alpha \) of the order of unity, the polaron radius in the low temperature limit has previously been calculated to be of the order of the healing length \( \xi \), justifying both our use of the low-momentum approximations \([5]\) and of the semiclassical approximation.

We believe, that the phenomena described above can be very conveniently measured in state-of-the-art experiments on ultracold fermion-boson mixtures. We envisage a dilute fermionic system being trapped in an optical lattice, which, in turn, is immersed into a BEC as is done in e. g. Refs. \([21,22]\). Assuming the interwell fermion hopping to be completely suppressed (for instance by making the lattice very deep) the lattice is then moved through the BEC at constant velocity. The fermions are then subject to a drag force, which can be measured as a population imbalance of the low-lying fermion states in the minimum of the potential well by a number of well established experimental techniques. Alternatively, after the transients die out, one can switch off the trapping potentials and infer the force from the velocity distributions of the freed particles.

From the theoretical point of view such an experiment is very convenient since the particle kinematics is fully known. Assuming the impurity/polaron to be a classical particle, the drag force is exactly given by the rhs of Eq. \((\ref{eq:6})\) under the condition \( r(t, u) = v_0(t - u) \), where \( v_0 \) is the drag velocity. The result of calculations is shown in the inset of Fig. \((\ref{fig:3})\). While in the subsonic case the asymptotic value of the force is zero, in the supersonic case some finite value is reached in the stationary situation \([25]\). Very interesting is the behavior of the drag force at \( t \to \infty \) as a function of \( v_0 \), which is given by the rhs of Eq. \((\ref{eq:8})\), see Fig. \((\ref{fig:3})\). It follows a \( 1/v_0^2 \) law just beyond the sound velocity with a finite value just above it. This is very different from the perturbative result \( \sim v_0^4 \) of the field theoretical computation, see e.g. \([18]\). Since a mechanical force can be interpreted as the amount of energy radiated per unit length, it is in fact more instructive to compare this to the famous result for Cherenkov radiation in classical electrodynamics by Frank and Tamm \([23]\), where this quantity scales as \( 1 - c^2/v_0^2 \), \( c \) being the velocity of light in a medium. Although in our case we have the same dependence on \( 1/v_0^2 \) which seems to be a feature of classical dynamics, the difference is that in the BEC case, we obtain an asymptotic decoupling from the bath for high velocities as well as the discontinuity at \( v_0 = c \). The latter feature is plausible, it is clearly a signature of the nonlinear polaron coupling mechanism since the discontinuity disappears if the coupling is linearized.

It would be very interesting to observe these effects in experiments. One possible realization could be \(^{6}\)Li fermionic impurities immersed into a BEC of \(^{23}\)Na \([7]\). In this setup the typical values for the force evaluate to \( F_\infty \approx 10^{-24} \text{ N} \) in conventional units. This corresponds to an impurity acceleration of the order of \( 10^4 \text{m/s}^2 \) and therefore seems to be well within reach of experimental observation \([7,22]\). As discussed above it might be advantageous to replace the usually used fermion impurities by heavier ones, or even bosonic ones like \(^{85}\)Rb. In this case the force would be of the order of \( 10^{-25} \text{ N} \).

To conclude, by means of the semiclassical approximation and its extensions we have investigated the dynamics of an impurity in a BEC and interacting with its Bogolyubov modes. It turns out to crucially depend on the velocity of the wave packet and is completely different in sub- and supersonic regimes. The resulting mechanical forces can be estimated and we expect them to be measurable in the upcoming experiments.

The authors would like to thank S. Maier, M. Oberthaler, T. Rentrop, T. Schuster, R. Scelle and A. Trautmann for many enlightening discussions. The authors are supported by the Centre of Quantum Dynamics and HGSFP of the University of Heidelberg.
[1] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. 80, 885 (2008).
[2] Q. Chen, J. Stajic, S. Tan, and K. Levin, Physics Reports 412, 1 (2005).
[3] I. Bloch, J. Dalibard, and S. Nascimbene, Nat Phys 8, 267 (2012).
[4] V. Gurarie and L. Radzihovsky, Annals of Physics 322, 2 (2007).
[5] R. P. Feynman, Statistical Mechanics: A Set Of Lectures, Advanced Book Classics (Westview Press, 1998).
[6] M. Bruderer, A. Klein, S. R. Clark, and D. Jaksch, Phys. Rev. A 76, 011605 (2007).
[7] J. Tempere, W. Casteels, M. K. Oberthaler, S. Knoop, E. Timmermans, and J. T. Devreese, Phys. Rev. B 80, 184504 (2009).
[8] A. Schirotzek, C.-H. Wu, A. Sommer, and M. W. Zwierlein, Phys. Rev. Lett. 102, 230402 (2009).
[9] C. J. M. Mathy, M. B. Zvonarev, and E. Demler, Nat. Phys. 8, 881 (2012).
[10] I. Carusotto, S. X. Hu, L. A. Collins, and A. Smerzi, Phys. Rev. Lett. 97, 260403 (2006).
[11] L. P. Pitaevskij and S. Stringari, Bose-Einstein Condensation, International Series of Monographs on Physics (Clarendon Press, 2000), repr. ed.
[12] H. Fröhlich, Adv. Phys. 3, 325 (1954).
[13] U. Weiss, Quantum Dissipative Systems, Series in Modern Condensed Matter Physics (World Scientific, 1999).
[14] A. Messiah, Quantum Mechanics (Dover Publications, 2000), unabr. repr. ed.
[15] F. M. Peeters and J. T. Devreese, Phys. Rev. B 32, 3515 (1985).
[16] A. O. Caldeira and A. J. Leggett, Physica A 121, 587 (1983).
[17] D. Dasenbrook, Master’s thesis, University of Heidelberg (2012).
[18] D. L. Kovrizhin and L. A. Maksimov, Phys. Lett. A 282, 421 (2001).
[19] A. Schmid, J. Low Temp. Phys. 49, 609 (1982).
[20] U. Eckern, G. Schön, and V. Ambegaokar, Phys. Rev. B 30, 6419 (1984).
[21] T. Schuster, Ph.D. thesis, University of Heidelberg (2012).
[22] T. Schuster, R. Scelle, A. Trautmann, S. Knoop, M. K. Oberthaler, M. M. Haverhals, M. R. Goosen, S. J. J. M. F. Kokkelmans, and E. Tiemann, Phys. Rev. A 85, 042721 (2012).
[23] I. Frank and I. Tamm, Compt. rend. de l’ Acad. Sci. U.R.S.S. 14, 109 (1937).
[24] This power law is different for systems of different dimensionalities.
[25] Due to a factorized system preparation at $t = 0$ and resulting polaron cloud formation process the force at intermediate times is finite. It roughly corresponds to the situation in which the impurity is ‘shot’ into the BEC from the outside.