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Bosonic heat bath associated with a moving soliton in a fermionic system

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Abstract. – When a soliton (such as a kink or vortex) in a condensed fermionic system moves, it produces particle-hole pairs. These approximately behave as a bosonic field, equivalent to a bath of harmonic oscillators and an effective bosonization of the fermion degrees of freedom very naturally arises. This work considers the theory of a moving soliton and an expression is given for the quantity, known as the spectral function, that characterises the effective bosons in the system. For a specific system possessing a soliton, the spectral function is evaluated.

A number of different condensed systems containing fermions possess long-range order which is characterised by a field known as the order parameter. In a mean-field approximation, the order parameter typically satisfies a non-linear equation that allows the existence of stable structures of finite spatial extent and we shall refer to these as "solitons." Some examples of solitons are given in the (by no means exhaustive) table below ([1]).

System	Fermions	Soliton
superconductors	electrons	line or pancake vortex
superfluid ^{3}He	^{3}He atoms	A-B phase boundary (a domain wall)
neutron star matter	neutrons	line vortex
the linear molecule trans-polyacetylene	electrons	kink interpolating between degenerate dimerization states

([1]) It is arguable whether the last entry in the table, polyacetylene, falls into the class of systems with long-range order. We have included it since the system is interesting in its own right and has added interest since its mathematical description is that of a "scalar kink", *i.e.* a one-dimensional *s*-wave superconductor with a real order parameter that interpolates between bulk-magnitude gaps of opposite sign.

Although significantly different mechanisms may produce the long-range order in these systems, they possess the common feature that the fermions are coupled to the soliton and any fluctuation or variations of the soliton are communicated to the fermions and vice versa. Furthermore, as far as many calculations go, the only significant features of these systems are the effective dimensionality of physical space and the tensor character of the order parameter. Thus an apparently diverse set of systems, with their associated solitons, may be covered by a single language and formalism.

The interaction of the soliton with the fermion degrees of freedom in the system is an important aspect to the problem, since motion of the soliton generally "stirs up" the fermions, producing particle-hole pairs which modify the dynamical behaviour of a "bare" soliton. We shall provide a quantum-mechanical treatment of both the soliton and the fermions and it will be shown that the particle-hole pairs act on the soliton as effective bosons, thus an approximate bosonization of the fermion degrees of freedom very naturally arises. It is the purpose of this work to characterize the interaction between the soliton in question and the effective bosonic degrees of freedom. We approach the problem via the partition function, which can be written as a functional integral over all realisations of the order parameter and whose integrand is of the form $\exp[-S]$ where S is a Euclidean action ([2]). We proceed in this way since it follows from work on dissipative quantum systems [1], [2], [3], that information, of direct relevance to dynamics, lies in the Euclidean action. Under reasonable assumptions, there is a non-local part of the effective action of a system at temperature $T \equiv \beta^{-1}$ that can be brought to the form

$$\frac{1}{2} \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_1 \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau_2 \, K(\tau_1 - \tau_2) \left[X(\tau_1) - X(\tau_2)\right]^2 , \tag{1}$$

where $X(\tau)$ is the position of the soliton as a function of the Euclidean time τ (τ is a variable introduced in the functional representation of the partition function) and $K(\tau)$ is a system-dependent kernel. A non-local effective action of this form was found by Caldeira and Leggett in their model of dissipation of a particle coupled to an environment of harmonic oscillators [1]. In the soliton problems at hand, the very existence of such a term in the Euclidean action allows the problem to be viewed as a system in which a "particle-like" object, the soliton, interacts with a *bosonic* field equivalent to a bath of harmonic oscillators ([3]).

We shall derive a non-local term of the type (1) from basic principles ([4]). More significantly, however, we extract the fundamental quantity that fully characterises the interaction of the soliton with the effective bosons in the problem; a quantity referred to as the *spectral function.*

To explain more, we note that in the work by Caldeira and Leggett, the part of the Euclidean Lagrangian involving the harmonic-oscillator heat bath and its coupling to the particle (with coordinate X) was $\sum_\alpha \left(m_\alpha \dot{y}_\alpha^2/2 + m_\alpha \omega_\alpha^2 y_\alpha^2/2 - c_\alpha y_\alpha X\right)$, where y_α are the oscillator coordinates and c_α are coupling constants. On "integrating" the oscillators out of the problem, it was found that their influence was encapsulated in $J(\omega) = \frac{\pi}{2} \sum_\alpha (c_\alpha^2/m_\alpha \omega_\alpha)\delta(\omega - \omega_a)$ and this quantity is known as the *spectral function.*

([2]) Throughout this work the constants $\hbar$ and k_B are taken to be unity; a prime, $'$, or an overdot, $\dot{}$, denote differentiation of a function with respect to x or τ; $\delta(x)$ and $\Theta(x)$ denote Dirac or Heaviside functions.

([3]) We note that a superconductor vortex was modelled as a point particle coupled to an oscillator heat bath in [4].

([4]) A fundamental paper studying the non-local effects of electrons on collective degrees of freedom was given in ref. [5]. Furthermore, in ref. [2] a non-local term in the effective action was derived for an ion in a normal Fermi liquid.

Here, we shall determine the corresponding spectral function, $J(\omega;T)$ that characterises the effective bosonic bath to which a soliton is coupled; we shall find this to be an explicitly temperature-dependent quantity.

We focus on a specific system where all calculations can be performed in closed form. This is valuable since most of the systems listed require a numerical treatment and with a solvable system we are able to explicitly determine the origin of any features found. The insight so gained may allow the understanding of numerical treatments of more complex systems.

The simplest of the solitons listed occurs in trans-polyacetylene (modelled as a continuum field theory [6]). In this system, the internal space is spanned by 2×2 matrices, the order parameter is real and the physical space is one-dimensional.

Despite the simplicity of this system, it is not atypical. It has the important feature, shared by all the other systems, that the soliton can trap the fermions in bound states as well as scattering them. We shall thus use polyacetylene as a prototypical example for our ideas on the dynamics of solitons.

The first quantized Hamiltonian for polyacetylene is [6] $H = v_{\mathrm{F}} p_x \sigma^3 + \Delta(x)\sigma^1$, where v_{F} is the Fermi velocity, p_x is the momentum operator associated with motion along the x-axis and $\sigma^{1,3}$ are Pauli matrices. The order parameter $\Delta(x)$ is real and depends on position and possibly time.

The partition function can be written as a functional integral over $\Delta(x;\tau)$:

$$Z = \oint\limits_{\Delta(x;-\beta/2)=\Delta(x;\beta/2)} \mathrm{d}[\Delta(x;\tau)] \exp\Big[-S_{\mathrm{f}}[\Delta(x;\tau)] - \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau \int \mathrm{d}x \Big(\frac{1}{g_1}\left[\Delta(x;\tau)\right]^2 + \frac{1}{g_2}\left[\partial_\tau \Delta(x;\tau)\right]^2 \Big) \Big], \tag{2}$$

where, up to an additive constant, the fermionic contribution to the action is ([5])

$$S_{\mathrm{f}}[\Delta(x;\tau)] \equiv -\mathrm{Tr}\ln\left(ip_0 + v_{\mathrm{F}} p_x \sigma^3 + \Delta(x;\tau)\sigma^1 \right). \tag{3}$$

The terms $\frac{1}{g_1}\int_{-\beta/2}^{\beta/2}\mathrm{d}\tau \int \mathrm{d}x\, [\Delta(x;\tau)]^2$ and $\frac{1}{g_2}\int_{-\beta/2}^{\beta/2}\mathrm{d}\tau \int \mathrm{d}x\, [\partial_\tau\Delta(x;\tau)]^2$ are associated with the potential and kinetic energies of the ions in the carbon chain and g_1 and g_2 are constants.

As it stands, the partition function, (2), is a formidably complicated quantity. We shall make a plausible physical approximation to the functional integral that corresponds to a semiclassical quantization of the motion of the soliton.

First, since solitons have very long-lived existence, we restrict the field configurations in (2) to those corresponding to a single soliton. This still leaves a complicated integral corresponding to all possible fluctuations about a soliton that do not take the field out of the one-soliton sector. We make the further assumption that, as far as the interaction with the fermions is

([5]) We use an operator formulation: thus p_0 is treated as an operator conjugate to τ and satisfies $[\tau, p_0] = i$, similarly $[x, p_x] = i$. Tr in (3) equals $\mathrm{Tr}_x \cdot \mathrm{Tr}_\tau$ where Tr_x denotes a trace, tr, over 2×2 matrix indices as well as a trace over the one-dimensional configuration space: $\mathrm{Tr}_x[\ldots] = \mathrm{tr}\int \mathrm{d}x \langle x|[\ldots]|x\rangle$ and Tr_τ denotes a trace over the eigenfunctions of p_0 which are required to be antiperiodic in τ over the interval of β. In the problem under consideration the fermions are non-interacting. For systems with non-trivial fermion-fermion interactions, $S_{\mathrm{f}}[\Delta(x;\tau)]$ should be replaced by the appropriate generalisation given in [7].

concerned, the soliton may be treated as a structure with a *rigid* shape whose only degree of freedom is its position (6), X.

With $\Delta_\mathrm{s}(x)$ the *equilibrium* shape of a *static* soliton located at the origin, the rigid soliton approximation entails, in (2), the replacements $\Delta(x) \to \Delta_\mathrm{s}(x - X(\tau))$,

$$\oint\limits_{\Delta(x;-\beta/2)=\Delta(x;\beta/2)} \mathrm{d}[\Delta(x;\tau)] \to \oint\limits_{X(-\beta/2)=X(\beta/2)} \mathrm{d}[X(\tau)] \quad \text{and leads to}$$

$$\begin{aligned}
Z &\simeq \oint\limits_{X(-\beta/2)=X(\beta/2)} \mathrm{d}[X(\tau)] \exp[-S_\mathrm{total}],\\
S_\mathrm{total} &= S_\text{mean field}[\Delta_\mathrm{s}(x)] + S_\mathrm{kinetic}[X(\tau)] + S_\text{non-local}[X(\tau)],\\
S_\text{mean field}\,[\Delta_\mathrm{s}(x)] &= S_\mathrm{f}\,[\Delta_\mathrm{s}(x)] + \frac{1}{g_1}\int\limits_{-\beta/2}^{\beta/2}\mathrm{d}\tau \int \mathrm{d}x\,[\Delta_\mathrm{s}(x)]^2\,, \qquad (4)\\
S_\mathrm{kinetic} &= \frac{1}{g_2}\int\limits_{-\beta/2}^{\beta/2}\mathrm{d}\tau\int\mathrm{d}x\left[\dot{X}(\tau)\Delta'_\mathrm{s}(x)\right]^2,\\
S_\text{non-local}[X(\tau)] &= S_\mathrm{f}\,[\Delta_\mathrm{s}(x - X(\tau))] - S_\mathrm{f}\,[\Delta_\mathrm{s}(x)]\,.
\end{aligned}$$

$\beta^{-1}\, S_\text{mean field}$ coincides with the mean-field free energy of a static soliton and $S_\text{non-local} + S_\mathrm{kinetic}$ are corrections to the static mean-field action.

S_total contains a non-local term of the form given in (1) as may be seen by expanding $S_\text{non-local}$ to quadratic order in X and we make the assumption that the higher-order terms may be neglected (7).

With $G^\mathrm{M}(\tau)$ the Matsubara Green's function appropriate to a static equilibrium soliton with Hamiltonian

$$H_\mathrm{s} = v_\mathrm{F} p_x \sigma^3 + \Delta_\mathrm{s}(x)\sigma^1\,, \qquad (5)$$

we find that the *quadratic* part of $S_\text{non-local}$ is

$$\begin{aligned}
S^{(2)}_\text{non-local}[X(\tau)] &= \frac{1}{2}\int\limits_{-\beta/2}^{\beta/2}\mathrm{d}\tau_1\int\limits_{-\beta/2}^{\beta/2}\mathrm{d}\tau_2 K(\tau_1-\tau_2)\,[X(\tau_1)-X(\tau_2)]^2\,,\\
K(\tau) &= -\frac{1}{2}\mathrm{Tr}_x\left[G^\mathrm{M}(\tau)\,\Delta'_\mathrm{s}(x)\sigma^1 G^\mathrm{M}(-\tau)\,\Delta'_\mathrm{s}(x)\sigma^1\right]. \qquad (6)
\end{aligned}$$

The presence of $S^{(2)}_\text{non-local}$ means Z has a non-local part of its action of the same form as that of Caldeira and Leggett [1] and we see a soliton coupled to a Fermi sea behaves as a point particle in contact with a bosonic bath.

(6) The position of a soliton is taken as an unambiguous feature of its profile; in polyacetylene we take this as the place where the order parameter vanishes.

(7) Terms in $S_\text{non-local}$ beyond second order in X correspond to anharmonicities of the effective oscillators and non-linear couplings to the soliton's coordinate.

Let us now consider the spectral function for the bosons, $J(\omega;T)$, analogous to that of Caldeira and Leggett [1]. In the work of these authors, the relationship between their kernel and spectral function was $K(\tau)=\int_0^\infty \frac{d\omega}{2\pi}J(\omega)\{\cosh[\omega(|\tau|-\beta/2)]\}/\sinh(\beta\omega/2)$. To find the spectral function in the soliton case, we use the key identity contained in the pair of equations [8]

$$\begin{cases} -\dfrac{1}{2}\mathrm{Tr}_x\left[G^{\mathrm{M}}(\tau)\,\Delta_{\mathrm{s}}'(x)\sigma^1 G^{\mathrm{M}}(-\tau)\,\Delta_{\mathrm{s}}'(x)\sigma^1\right]=\displaystyle\int_0^\infty \frac{d\omega}{2\pi}J(\omega;T)\frac{\cosh[\omega(|\tau|-\beta/2)]}{\sinh(\beta\omega/2)}\,, \\ J(\omega;T)=\tanh(\beta\omega/2)\,\mathrm{Re}\left\{\displaystyle\int_{-\infty}^{\infty}dt\,\cos(\omega t)\mathrm{Tr}_x\left[G^{\mathrm{T}}(t)\,\Delta_{\mathrm{s}}'(x)\sigma^1 G^{\mathrm{T}}(-t)\,\Delta_{\mathrm{s}}'(x)\sigma^1\right]\right\}, \end{cases} \tag{7}$$

in which $G^{\mathrm{T}}(t)$ is the equilibrium *time-ordered* Green's function for H_{s}. A comparison of (6) and (7) indicates that $J(\omega;T)$ of (7) constitutes an explicit expression for the spectral function in terms of equilibrium quantities and there are natural generalisations of this result to other systems.

Evaluation of $J(\omega;T)$ requires a knowledge of the soliton profile appearing in H_{s}. Following [6] we take $\Delta_{\mathrm{s}}(x)=\Delta_0\tanh\left(\frac{x}{v_{\mathrm{F}}/\Delta_0}\right)$, where Δ_0 is the bulk order parameter and we are able to obtain exact results for $J(\omega;T)$. Here we have space only to state the results in particular limits.

At zero temperature a contribution arises only from transitions between bound and scattering states and the gap in the spectrum between these states is manifested by the vanishing of $J(\omega;0)$ for $\omega<\Delta_0$:

$$J(\omega;0)=\frac{\pi^2}{32}\frac{\Delta_0}{\xi_0^2}\left(\frac{\omega}{\Delta_0}\right)^5\mathrm{sech}^2\left(\frac{\pi}{2}\sqrt{\left(\frac{\omega}{\Delta_0}\right)^2-1}\right)\frac{\Theta\left(\left(\frac{\omega}{\Delta_0}\right)^2-1\right)}{\sqrt{\left(\frac{\omega}{\Delta_0}\right)^2-1}}\,. \tag{8}$$

The gap in the in the spectrum suggests that the long-time soliton dynamics at zero temperature may be governed by other processes, involving a low-frequency component.

At low temperatures, the low-frequency behaviour of $J(\omega;T)$ arises only from transitions between states with closely spaced eigenvalues: in the system considered these are only scattering states. We find

$$J(\omega;T)\underset{\substack{\omega\ll\Delta_0\\ \beta\Delta_0>1}}{\simeq}\frac{\pi}{8}\frac{\Delta_0}{\xi_0^2}\left(\frac{\omega}{\Delta_0}\right)^2\sinh(\beta\omega/2)E_2(\beta\Delta_0)\,, \tag{9}$$

with $E_2(\alpha)\equiv\int_1^\infty y^{-2}\exp[-\alpha y]dy$ and corrections to the above formula are of relative order $O\left((\omega/\Delta_0)^2\ln(\beta\omega)\right)$ or $O\left((\omega/\Delta_0)^2\right)$.

Generally, the spectral function is an important ingredient in the dynamics of solitons, since properties such as their dissipation, mass, diffusion and tunnel escape-rate are governed by this quantity [9]. This work contains a direct route by which the spectral function may be determined and further details of the calculations and applications to other systems will be published elsewhere.

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[8] A proof of this identity, based on a spectral decomposition of the Green's functions, will be given elsewhere.

[9] Recent work on the motion of domain walls in magnetic materials in which a spectral density is calculated and applied is that of ref. [8].

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