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The free energy of solitons coupled to fermions: absence of a gradient expansion at zero temperature due to bound states

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Abstract. Polyacetylene, regarded as one of the simplest systems bearing solitons which are coupled to fermions, is investigated at zero temperature. With λ denoting the soliton size in units of the coherence length, solitons with $\lambda \gg 1$ are considered. It is found, from the exact results of Nakahara *et al* (for a hyperbolic tangent soliton profile), that the soliton creation energy does not possess an expansion in powers of $1/\lambda$, as would be expected of a gradient expansion. Rather, the leading terms in a large-λ expansion are found to be $a\lambda + b\lambda^{-1/2}$ with constant a and b. Calculations are presented for general soliton profiles. They show that the term linear in λ is the soliton creation energy to zeroth order in gradients. The term $b\lambda^{-1/2}$ is shown to arise purely from bound states of the fermions (electrons) trapped by the soliton. The evaluation of the coefficient b requires the extraction of the finite difference between a divergent sum and integral, a procedure employed in the Casimir effect.

1. Introduction

One of the simplest examples of a condensed matter system that contains fermions and has the ability to support topological solitons is the linear molecule polyacetylene. From the lessons learned from an exactly soluble model of this system, we believe a number of general features of other, soliton-bearing, fermionic systems may be inferred.

The low-energy physics of polyacetylene, appropriate to this work, is that of a chain of atomic sites, carbon ions, along which electrons hop; one electron being denoted by each carbon atom in the chain. The interaction of the electrons with the carbon chain results in it being energetically favourable for the carbon chain to acquire a dimerization (i.e. a staggered displacement). The pairings associated with this dimerization can occur in two different ways and result in two degenerate ground states that are characterized by dimerizations of opposite sign. A topological soliton in polyacetylene is an interpolation of the dimerization from one of these degenerate ground states to the other and occurs over a finite spatial distance.

At zero temperature, the case we shall principally concentrate on in this work, the soliton is partially characterized by the excess energy a soliton-bearing system has over a uniform system. We term this energy the soliton creation energy.

The objective of the present work is to investigate the behaviour of the soliton creation energy when the soliton has a spatial extent that is large compared with the coherence length in the problem, ξ_0.

In section 2 of this work we derive a form for the soliton creation energy for general soliton profiles when the dimerization is treated as a static field. Section 3 obtains an

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expansion of the soliton creation energy for large solitons. In section 4 it is shown that the gradient expansion breaks down at the second non-zero term in the expansion and, in section 5, we provide a method to calculate the second term in the large-scale expansion from purely bound state contributions. Section 6 consists of a discussion. There are two appendices.

We shall work in units in which $\hbar = 1$ and use a prime symbol to denote differentiation of any function with respect to its argument.

2. General expression for the soliton creation energy

Much of the material in this section can be found in greater detail in section 3 and the related appendix of [1]. The model of polyacetylene we consider consists of a continuum field theory of fermions moving in one spatial dimension (labelled by x) and coupled to a static dimerization field $\Delta(x)$ [2]. Denoting the free energy of the soliton-bearing system by F and that of the uniformly dimerized system by F_0 the quantity $F - F_0$ may be expressed solely as a functional of $\Delta(x)$. This arises as follows. Let ψ and $\bar{\psi}$ be independent Grassmann fields which are functions of the Euclidean time variable τ and are antiperiodic in this variable over the interval β (the inverse temperature). Then we can write

$$e^{-\beta(F-F_0)} = \frac{\int \mathrm{d}\bar{\psi}\,\mathrm{d}\psi\, \exp(-\int_0^\beta \mathrm{d}\tau \int \mathrm{d}x\, \bar{\psi}(\partial_\tau + H)\psi)}{\int \mathrm{d}\bar{\psi}\,\mathrm{d}\psi\, \exp(-\int_0^\beta \mathrm{d}\tau \int \mathrm{d}x\, \bar{\psi}(\partial_\tau + H_0)\psi)}\, e^{-\beta\Omega \int \mathrm{d}x(\Delta^2 - \Delta_0^2)} \tag{2.1a}$$

where

$$H = -\mathrm{i}v_{\mathrm{F}}\partial_x\sigma_3 + \Delta(x)\sigma_1 \tag{2.1b}$$

$$H_0 = -\mathrm{i}v_{\mathrm{F}}\partial_x\sigma_3 + \Delta_0\sigma_1 \tag{2.1c}$$

Ω is a combination of spring and coupling constants (that need not concern us here). σ_k $(k = 1, 2, 3)$ are the Pauli matrices; they describe the physics of electrons moving at $\pm$ the Fermi velocity v_{F}. The quantities $\Delta(x)$ and Δ_0 indicate dimerization in the presence of the soliton and in the uniform system, respectively. The electronic spin merely results in a factor of two appearing in the free energy. The functional integrals can be carried out and yield a ratio of two functional determinants, thus

$$F - F_0 = -\frac{2}{\beta}\ln\left(\frac{\mathrm{Det}[\partial_\tau + H]}{\mathrm{Det}[\partial_\tau + H_0]}\right) + \Omega \int \mathrm{d}x(\Delta^2 - \Delta_0^2) \tag{2.2}$$

where the factor of two results from the two spin contributions. It is convenient at this stage to diagonalize ∂_τ (eigenvalues $\mathrm{i}\omega_m = \mathrm{i}(2m+1)\pi/\beta$, $m = 0, \pm1, \pm2, \ldots$) and to combine the contributions of ω_m and $-\omega_m$ (with a requisite factor of $\frac{1}{2}$ in front of the logarithm). With 'det' denoting the determinant taken over reduced space where the eigenfunctions depend only on x and Pauli indices, we obtain

$$F - F_0 = -\frac{1}{\beta}\sum_m \ln\left(\frac{\det[\omega_m^2 + H^2]}{\det[\omega_m^2 + H_0^2]}\right) + \Omega \int \mathrm{d}x(\Delta^2 - \Delta_0^2). \tag{2.3}$$

The soliton creation energy is the zero-temperature limit of $F - F_0$, and we denote this quantity by $E - E_0$. In this limit the Matsubara frequency sum goes into an integral over frequency. Furthermore, a convenient form for $E - E_0$ is obtained by (i) using the identity ln det ≡ Tr ln (Tr denotes the trace in the space with spatial and matrix degrees of freedom) and (ii) using the fact that $F - F_0$ is stationary variations of the uniform dimerization Δ_0 at fixed Δ. It may be verified that the stationarity requirement results in

$$\frac{1}{\beta}\sum_m \mathrm{Tr}\frac{1}{\omega_m^2 + H_0^2} = \Omega \int \mathrm{d}x. \tag{2.4}$$

Using this equation we obtain the following result for the soliton creation energy which is a functional of $\Delta(x)$ and applies for general soliton profiles:

$$E - E_0 = -\int \frac{\mathrm{d}\omega}{2\pi}\mathrm{Tr}\left[\ln\left(\frac{\omega^2 + H^2}{\omega^2 + H_0^2}\right) - \frac{1}{\omega^2 + H_0^2}(H^2 - H_0^2)\right]. \tag{2.5}$$

In later sections we shall find it convenient to go over to a more general operator picture. Thus, we regard the trace in equation (2.5) as being taken over the abstract space spanned by kets $|x\rangle$ (matrix indices will be suppressed). The appropriate operators in this space are the momentum and coordinate operators p and x, respectively. (To go to this operator picture we must replace $-\mathrm{i}\partial_x$ in, for example, equation (2.1*b*) by p.) To avoid possible confusion between operators and *c*-numbers we shall reserve the symbol p only for momentum operators.

3. Exact results for the expansion of the soliton creation energy for large solitons

In [3] an exact representation of the soliton creation energy was obtained when the soliton profile was a hyperbolic tangent (tanh). The soliton profile adopted was

$$\Delta(x) = \Delta_0 \tanh\left(\frac{x}{\lambda\xi_0}\right) \tag{3.1}$$

where λ is a dimensionless parameter characterizing the soliton size and the coherence length ξ_0 is given in terms of the uniform dimerization and Fermi velocity by

$$\xi_0 = \frac{v_F}{\Delta_0}. \tag{3.2}$$

For the analysis of the present section, the most convenient expression for the soliton creation energy was given in [1]:

$$\frac{E - E_0}{\Delta_0} = 1 + \frac{2}{\pi}\Psi(\lambda) \tag{3.3a}$$

$$\Psi(\lambda) = \int_0^\infty \mathrm{d}t\, K_1(t)\left(\frac{4\sinh^2(t/2)}{t}\frac{1}{\mathrm{e}^{t/\lambda} - 1} - \lambda\right) \tag{3.3b}$$

where K_1 is a Bessel function of imaginary argument of order 1 [4].

The naive way to proceed in the limit of large λ is to expand the exponential:

$$\frac{1}{\mathrm{e}^{t/\lambda} - 1} = \frac{\lambda}{t} - \frac{1}{2} + \frac{1}{12}\left(\frac{t}{\lambda}\right) + \mathrm{O}\left[\left(\frac{t}{\lambda}\right)^2\right]. \tag{3.4}$$

This leads to

$$\frac{E-E_0}{\Delta_0}=A\lambda+B+C/\lambda+\dots \tag{3.5a}$$

$$A=\frac{2}{\pi}\int_0^\infty \mathrm{d}t\,K_1(t)\left(\frac{4\sinh^2(t/2)}{t^2}-1\right) \tag{3.5b}$$

$$B=1-\frac{1}{\pi}\int_0^\infty \mathrm{d}t\,K_1(t)\,\frac{4\sinh^2(t/2)}{t} \tag{3.5c}$$

$$C=\frac{1}{6\pi}\int_0^\infty \mathrm{d}t\,K_1(t)4\sinh^2\left(\frac{t}{2}\right). \tag{3.5d}$$

Note that for large t we have [4]

$$K_1(t)\sim\sqrt{\frac{\pi}{2t}}\,\mathrm{e}^{-t} \tag{3.6}$$

and it immediately follows that A and B are well defined but C diverges due to the slow speed of vanishing of the integrand

$$C\sim\int^\infty \mathrm{d}t\,t^{-1/2} \tag{3.7}$$

and higher terms in the expansion of equation (3.5) will be progressively more divergent due to the increased powers of t present.

The above indicates that more careful considerations must be given to the terms containing negative powers of λ. If we note that for $t\geqslant\lambda$, the exponential comes into play and cuts off the integrand, it seems likely that the leading term in negative powers of λ is $\mathrm{O}(\lambda^{-1/2})$ rather than $\mathrm{O}(\lambda^{-1})$.

To verify this we write, with no approximation,

$$\frac{E-E_0}{\Delta_0}=A\lambda+B+\chi(\lambda) \tag{3.8a}$$

$$\chi(\lambda)=\frac{2}{\pi}\int_0^\infty \mathrm{d}t\,K_1(t)\,\frac{4\sinh^2(t/2)}{t}\left(\frac{1}{\mathrm{e}^{t/\lambda}-1}-\frac{\lambda}{t}+\frac{1}{2}\right). \tag{3.8b}$$

The coefficients A and B may be exactly determined if the representation

$$K_1(t)=t\int_1^\infty \mathrm{d}u(u^2-1)^{1/2}\,\mathrm{e}^{-ut} \tag{3.9}$$

is used for the Bessel function [4] and the t integration is carried out first. The result is ($\zeta(x)$ is the Riemann zeta function)

$$A=\frac{3}{2\pi}(2-\zeta(2))\simeq 0.170 \tag{3.10a}$$

$$B=0. \tag{3.10b}$$

In appendix 1 the leading behaviour of the function $\chi(\lambda)$ is extracted:

$$\begin{aligned}\chi(\lambda)&=\frac{\zeta(\frac{3}{2})}{\sqrt{2}\pi}\frac{1}{\sqrt{\lambda}}+\mathrm{O}(\lambda^{-1})\\&\simeq 0.588\lambda^{-1/2}+\mathrm{O}(\lambda^{-1}).\end{aligned} \tag{3.11}$$

We thus find that the exact result for the hyperbolic tangent soliton profile leads to the large-λ expansion

$$\frac{E-E_0}{\Delta_0}=\frac{3}{2\pi}(2-\zeta(2))\lambda+\frac{\zeta(\frac{3}{2})}{\sqrt{2}\pi}\frac{1}{\sqrt{\lambda}}+O(\lambda^{-1})$$

$$\simeq 0.170\lambda+0.588\lambda^{-1/2}+O(\lambda^{-1}). \tag{3.12}$$

4. Breakdown of the gradient expansion of the soliton creation energy

In this section we show that the gradient expansion, when applied to the general result for the soliton creation energy, breaks down at a finite order.

We have, from equation (2.5), the result for the soliton creation energy:

$$\frac{E-E_0}{\Delta_0}=-\frac{1}{\Delta_0}\int\frac{d\omega}{2\pi}\mathrm{Tr}\left[\ln\left(\frac{\omega^2+v_F^2p^2+\Delta^2(x)+\sigma_2 v_F\Delta'(x)}{\omega^2+v_F^2p^2+\Delta_0^2}\right)-\frac{\Delta^2(x)-\Delta_0^2}{\omega^2+v_F^2p^2+\Delta_0^2}\right]. \tag{4.1}$$

We assume a soliton profile that is given by

$$\Delta(x)=\Delta_0\Phi\left(\frac{x}{\lambda\xi_0}\right) \tag{4.2}$$

where $\Phi(x)$ is taken to be an odd, monotonically increasing function that approaches ± 1 at spatial infinity:

$$\Phi(\pm\infty)=\pm 1. \tag{4.3}$$

λ is a measure of the soliton size in units of the coherence length ξ_0 (which was given in equation (3.2)).

Proceeding, let us now perform the canonical transformation

$$x\to\frac{\lambda v_F}{\Delta_0}x \qquad p\to\frac{\Delta_0}{\lambda v_F}p \tag{4.4}$$

within the trace of equation (4.1). Since this transformation preserves the commutation relation $[x,p]=i$, it leaves the trace invariant. Furthermore, on rescaling ω,

$$\omega=\Delta_0\nu \tag{4.5}$$

we obtain

$$\frac{E-E_0}{\Delta_0}=-\int\frac{d\nu}{2\pi}\mathrm{Tr}\left[\ln\left(\frac{\nu^2+p^2/\lambda^2+\Phi^2(x)+\sigma_2\Phi'(x)/\lambda}{\nu^2+p^2/\lambda^2+1}\right)-\frac{\Phi^2(x)-1}{\nu^2+p^2/\lambda^2+1}\right]. \tag{4.6}$$

Next, we use the result, valid for any function f of coordinate and momentum operators that possess a finite trace (tr denotes the trace over the matrix indices),

$$\mathrm{Tr}\,f(x,p)=\mathrm{tr}\int\frac{dk\,dx}{2\pi}f(x,k-i\partial_x). \tag{4.7}$$

A proof of this result is given in appendix 2. Lastly, the change of variables corresponding to the rescaling $k\to\lambda k$ gives a form for $(E-E_0)/\Delta_0$ that is suitable for a gradient expansion ($\sigma=\pm1$ are the eigenvalues of σ_2):

$$\frac{E-E_0}{\Delta_0}=-\lambda\int\frac{\mathrm{d}\nu\,\mathrm{d}k\,\mathrm{d}x}{(2\pi)^2}$$
$$\times\sum_{\sigma=\pm1}\left[\ln\left(\frac{\nu^2+k^2+\Phi^2(x)-(2\mathrm{i}k/\lambda)\partial_x-(\partial_x^2/\lambda^2)+(\sigma\Phi'(x)/\lambda)}{\nu^2+k^2+1}\right)\right.$$
$$\left.-\frac{\Phi^2(x)-1}{\nu^2+k^2+1}\right]. \tag{4.8}$$

In this last form, each derivative comes with a power of λ^{-1}, thus, if it exists, an expansion in powers of derivatives is equivalent to an expansion in powers of λ^{-1}.

The leading term in a derivative expansion follows by setting $\lambda^{-1}=0$ within the integrals. This yields

$$\frac{(E-E_0)^{(0)}}{\Delta_0}=-\lambda\int\frac{\mathrm{d}\nu\,\mathrm{d}k\,\mathrm{d}x}{(2\pi)^2}2\left[\ln\left(\frac{\nu^2+k^2+\Phi^2}{\nu^2+k^2+1}\right)-\frac{\Phi^2-1}{\nu^2+k^2+21}\right]$$
$$=\frac{\lambda}{\pi}\int_0^\infty\mathrm{d}x\left[(1-\Phi^2(x))+2\Phi^2(x)\ln\Phi(x)\right]. \tag{4.9}$$

The exact results given in section 3 hold for the soliton profile $\Phi(x)=\tanh(x)$. If this is substituted into equation (4.9) the result is obtained in accordance with equations (3.8*a*) and (3.10*a*). We thus see that the term in the soliton creation energy that is linear in λ arises simply from the neglect of gradients: it is the contribution from the system adiabatically adjusting to the slowly varying soliton profile. The absence of derivatives and hence of commutators indicates that this is a result that follows from classical, i.e. non-quantum, considerations.

Higher terms in the gradient expansion follow from expansion of the logarithm according to

$$\ln(A+B)=\ln A+\ln(1+A^{-1}B)$$
$$=\ln A+A^{-1}B-\tfrac{1}{2}(A^{-1}B)^2+\dots \tag{4.10}$$

where A is chosen to be $\nu^2+k^2+\Phi^2(x)$. It immediately follows that there are no terms of $\mathrm{O}(\lambda^0)$ since this contribution has an integrand that is odd under $k\to-k$ and $\sigma\to-\sigma$.

The term of $\mathrm{O}(\lambda^{-1})$ that would be expected to follow in a gradient expansion may, straightforwardly, be shown to be

$$\frac{1}{2\lambda}\int\frac{\mathrm{d}\nu\,\mathrm{d}k\,\mathrm{d}x}{(2\pi)^2}\sum_{\sigma=\pm1}\frac{1}{(\nu^2+k^2+\Phi^2(x))^2}(\Phi'(x))^2=\frac{1}{2\pi\lambda}\int_0^\infty\mathrm{d}x\left(\frac{\Phi'(x)}{\Phi(x)}\right)^2. \tag{4.11}$$

For $\Phi(x)$ approaching zero as any non-zero power of x (recall it is odd), results in an integrand behaving as x^{-2} for small x and thus the integral diverges. In this way we see that the gradient expansion breaks down at the term of second order in gradients due to the vanishing of the soliton profile. This is a fundamental breakdown since the vanishing of the dimerization is a necessary condition for the very existence of a soliton!

The results of this section indicate that the absence of an expansion of the soliton creation energy in powers of λ^{-1} is not a special feature of the hyperbolic tangent profile but a feature present for general soliton profiles.

5. Determination of the $\lambda^{-1/2}$ term in the soliton creation energy and its physical origin

In section 4 we attempted to use a gradient expansion to generate a series for the soliton creation energy in powers of λ^{-1}. We found that no such expansion was possible and the procedure, despite applying to general soliton profiles, mirrored (albeit in a very different language) the calculation for the hyperbolic tangent profile given in section 3. Let us pursue this analogy in this section and write equation (4.8) in the suggestive form

$$\frac{E-E_0}{\Delta_0}=-\lambda\int\frac{\mathrm{d}\nu\,\mathrm{d}k\,\mathrm{d}x}{(2\pi)^2}2\left[\ln\left(\frac{\nu^2+k^2+\Phi^2}{\nu^2+k^2+1}\right)-\frac{\Phi^2-1}{\nu^2+k^2+1}\right]+\chi(\lambda) \tag{5.1a}$$

where

$$\chi(\lambda)=-\int\frac{\mathrm{d}\nu\,\mathrm{d}k\,\mathrm{d}x}{(2\pi)^2}\left(\sum_\sigma\ln\left(\nu^2+k^2+\Phi^2\left(\frac{x}{\lambda}\right)-2\mathrm{i}k\partial_x-\partial_x^2+\frac{\sigma\Phi'(x/\lambda)}{\lambda}\right)\right.$$
$$\left.-2\ln\left(\nu^2+k^2+\Phi^2\left(\frac{x}{\lambda}\right)\right)\right) \tag{5.1b}$$

(and we have made the change of variables equivalent to the rescaling $x\to x/\lambda$). The leading term in equation (5.1a) has been dealt with in section 4 and we now concentrate on equation (5.1b) for $\chi(\lambda)$.

Individually, the contribution from each of the logarithms in equation (5.1b) diverges and, thus, both logarithms should be treated together. To properly treat them separately requires the imposition of a suitable cut-off which makes the individual contributions finite. Only when the two contributions are combined should the cut-off be allowed to tend to infinity. We shall not do this here but, rather, shall naively manipulate the two contributions separately. The principal reasons for our approach are simplicity of treatment and the naturalness of the final expression. Our manipulations also lead to the exact result.

To proceed, we re-express the k, x integral over the leading logarithm of equation (5.1b) in terms of a trace over operators p and x (i.e. we use equation (4.7) from right to left). We obtain

$$\chi(\lambda)=-\int\frac{\mathrm{d}\nu}{2\pi}\left\{\mathrm{Tr}\left[\ln\left(\nu^2+p^2+\Phi^2\left(\frac{x}{\lambda}\right)+\frac{\sigma_2\Phi'(x/\lambda)}{\lambda}\right)\right]\right.$$
$$\left.-2\int\frac{\mathrm{d}k\,\mathrm{d}x}{2\pi}\ln\left(\nu^2+k^2+\Phi^2\left(\frac{x}{\lambda}\right)\right)\right\}. \tag{5.2}$$

Our approximation, which aims to capture the leading λ dependence of $\chi(\lambda)$ is to replace Φ by its linear approximation

$$\Phi\left(\frac{x}{\lambda}\right)=\frac{x}{\lambda}\Phi'(0). \tag{5.3}$$

This assumes a smooth soliton profile and uses the vanishing of Φ at the origin. It seems additionally appropriate since: (i) λ is large and hence x/λ is 'small' in an average sense; (ii) the small-argument behaviour of $\Phi(x)$ results in the gradient expansion breaking down. An accurate treatment of the small-argument behaviour therefore seems the most natural direction to proceed. Thus, the function obtained from the linearlized profile is denoted by $\chi_L(\lambda)$ and is given by

$$\chi_L(\lambda) = -\int \frac{d\nu}{2\pi}\left\{\mathrm{Tr}\left[\ln\left(\nu^2+p^2+\frac{[\Phi'(0)]^2x^2}{\lambda^2}+\frac{\sigma_2\Phi'(0)}{\lambda}\right)\right]\right.$$
$$\left. -2\int \frac{dk\,dx}{2\pi}\ln\left(\nu^2+k^2+\frac{[\Phi'(0)]^2}{\lambda^2}x^2\right)\right\}. \tag{5.4}$$

Defining

$$\omega = 2|\Phi'(0)|/\lambda \tag{5.5}$$

we see that the operator appearing in equation (5.4) is that of a simple harmonic oscillator of mass $\frac{1}{2}$ and angular frequency ω. Thus, the trace in equation (5.4) becomes

$$\mathrm{Tr}\left[\ln\left(\nu^2+p^2+\frac{\omega^2x^2}{4}+\frac{\sigma_2\omega}{2}\right)\right] = \sum_{n=0}^{\infty}\sum_{\sigma=\pm1}\ln\left(\nu^2+(n+\tfrac{1}{2})\omega+\frac{\sigma\omega}{2}\right). \tag{5.6}$$

On going to appropriately scaled coordinates in the k, x plane, the second term involving the logarithm in equation (5.4) can be written:

$$2\int \frac{dk\,dx}{2\pi}\ln\left(\nu^2+k^2+\frac{\omega^2x^2}{4}\right) = 2\int_0^\infty dn\,\ln(\nu^2+n\omega). \tag{5.7}$$

Thus, equation (5.4) can be written as

$$\chi_L(\lambda) = -\int \frac{d\nu}{2\pi}\left[\left(\sum_{n=1}^{\infty}-\int_0^\infty dn\right)+\left(\sum_{n=0}^{\infty}-\int_0^\infty dn\right)\right]\ln(\nu^2+n\omega). \tag{5.8}$$

Following the work of [5], where the extraction of the finite difference between a divergent sum and a divergent integral is given, we define Σ' by

$$\sum_{n=0}^{\infty}{}' f(n) = \tfrac{1}{2}f(0) + \sum_{n=1}^{\infty} f(n). \tag{5.9}$$

We can then write

$$\chi_L(\lambda) = -2\int \frac{d\nu}{2\pi}\left(\sum_{n=0}^{\infty}{}'-\int_0^\infty dn\right)\ln(\nu^2+n\omega). \tag{5.10}$$

Noting that the results of [5] imply

$$\left(\sum_{n=0}^{\infty}{}'-\int_0^\infty dn\right)\times\text{constant} = 0 \tag{5.11}$$

we have

$$\chi_L(\lambda) = -2\int \frac{d\nu}{2\pi}\left(\sum_{n=0}^{\infty}{}'-\int_0^\infty dn\right)\ln\left(\frac{\nu^2}{\omega}+n\right). \tag{5.12}$$

The difference between the divergent sum and integral appearing in this equation is given in equation (5.2) of [5]:

$$\left(\sum_{n=0}^{\infty}{}'-\int_0^\infty dn\right)\ln(\eta+n) = -[\ln\Gamma(\eta)-(\eta-\tfrac{1}{2})\ln\eta+\eta-\tfrac{1}{2}\ln 2\pi]. \tag{5.13}$$

We find that $\chi_L(\lambda)$ may be written as

$$\chi_L(\lambda)=\sqrt{\frac{2|\Phi'(0)|}{\lambda}}\,\frac{2}{\pi}\int_0^\infty d\nu[\ln\Gamma(\nu^2)-(\nu^2-\tfrac{1}{2})\ln\nu^2+\nu^2-\tfrac{1}{2}\ln 2\pi]. \tag{5.14}$$

The integral may be evaluated in closed form by using the representation [4]

$$\ln\Gamma(z)=(z-\tfrac{1}{2})\ln z-z+\tfrac{1}{2}\ln 2\pi+2\int_0^\infty dt\frac{\tan^{-1}(t/z)}{e^{2\pi t}-1}. \tag{5.15}$$

This leads to

$$\chi_L(\lambda)=4\int\frac{d\nu}{2\pi}\int_0^\infty dt\frac{\tan^{-1}(\omega t/\nu^2)}{e^{2\pi t}-1}. \tag{5.16}$$

Then the change of variables $\nu\to(t/u)^{1/2}$ decouples the two integrals and leads to

$$\chi_L(\lambda)=\frac{\zeta(3/2)}{2\pi}\sqrt{\omega}\equiv\frac{\zeta(\frac{3}{2})}{\sqrt{2}\pi}\frac{|\Phi'(0)|}{\sqrt{\lambda}}. \tag{5.17}$$

When $|\Phi'(0)|=1$, this result coincides exactly with the result found for the hyperbolic tangent profile, equation (3.12). The linearization of the soliton profile, equation (5.3), is thus seen to account for the entire $\lambda^{-1/2}$ dependence in the large-λ expansion.

Let us enquire about the physical origin of the $\lambda^{-1/2}$ term in the soliton creation energy. Looking back to section 2 of this paper, it is evident that the logarithms in the free energy originated from an explicit 'integration out' of the electrons in the problem. The eigenvalues of the frequency-independent part of the argument of the logarithm may then be identified with the electronic spectrum. It follows that the discrete part of the spectrum is associated with bound states of the electrons localized in the vicinity of the soliton. The $\lambda^{-1/2}$ term in the soliton creation energy is thus seen to be a measure of a spectral weight difference, namely that of the excitation spectrum in the presence of the soliton and that following from the semiclassical estimate found by neglecting derivitives. In contrast to the leading, linear, term in the soliton creation energy, the $\lambda^{-1/2}$ term has an intrinsically quantum mechanical nature—there being no notion of discrete numbers associated with bound particles in classical mechanics.

6. Discussion

In this work an expansion of the soliton creation energy has been investigated. The leading terms in an expansion of the soliton creation energy for large values of the dimensionless soliton size λ were found (i) for a specific soliton profile and then (ii) for general soliton profiles. An expansion of the form $a\lambda+b\lambda^{-1/2}+\ldots$ was found, indicating the absence of a gradient expansion, irrespective of how large the soliton is. The term of $O(\lambda^{-1/2})$, which signalled the non-existence of a gradient expansion, was shown to originate from bound states of electrons on the soliton. The calculation of the coefficient of $\lambda^{-1/2}$ required the extraction of the finite difference between a sum over the bound state contributions and an integral over a semiclassical phase space estimate. It is interesting that such techniques were developed in the Casimir effect where discrete and continuous mode contributions have to be subtracted and we wonder whether there exist any deeper connections or analogies between soliton physics and the Casimir effect.

The present work has dealt only with the case of zero temperature. For the part of the soliton creation energy that is linear in λ, it is straightforward to obtain the finite-temperature extension by replacing the frequency integral by a sum over Matsubara frequencies (we shall leave it implicitly understood in what follows that the finite-temperature value of the uniform dimerization Δ_0 is used in all formulae). The above generalization to finite temperatures still results in a contribution that is linear in λ.

Consider next the terms that are corrections to the term linear in λ. These are given by equation (5.2). We can see some of the finite-temperature corrections by continuing to work with the linearized profile whose contribution is given in equation (5.16) by $\chi_L(\lambda)$. By replacing the frequency integral by a Matsubara sum and employing the Poisson summation trick it can be shown that the leading correction to the zero-temperature part of $\chi_L(\lambda)$ is $O[1/(\beta\Delta_0)]$. Thus, providing the temperature is sufficiently low that $\beta\Delta_0$ is large compared with unity, the zero-temperature part will be the dominant term. We can see the range of temperatures where the gradient expansion is applicable by expanding in powers of λ^{-1}. This is most easily achieved by expanding the inverse tangent term in equation (5.16). It is seen that the expansion parameter is proportional to $\lambda^{-1}(\beta\Delta_0)^2$. This will be small in the Ginzburg–Landau regime where Δ_0 is small, i.e. close to the transition temperature. In polyacetylene the extremely high transition temperature makes this temperature region uninteresting; however, in systems with a similar mathematical description, such as superconductors, it is a region of considerable interest.

The results for the soliton creation energy presented in this work are valid when λ is large compared with unity. It is interesting to enquire whether they furnish a reasonable description even when λ is not large. From [11] we know that the exact soliton creation energy for a hyperbolic tangent profile is given by

$$\lambda = 1 \qquad \frac{E-E_0}{\Delta_0} = \frac{2}{\pi} \qquad \text{exact.} \tag{6.1}$$

If we use the approximate form obtained by keeping the leading two terms in the large-λ expansion, equation (3.12),

$$\left(\frac{E-E_0}{\Delta_0}\right) \simeq 0.170\lambda + 0.588\lambda^{-1/2} \tag{6.2}$$

and minimize with respect to λ we find

$$\lambda \simeq 1.441 \qquad \frac{E-E_0}{\Delta_0} \simeq 0.735 \qquad \text{approximate.} \tag{6.3}$$

These correspond to errors in λ and $(E-E_0)/\Delta_0$ of 44% and 15%, respectively.

Finally, let us comment on the relevance of the methods presented in this paper to other soliton-bearing fermionic systems. Any system described by a mean field type of second quantized Hamiltonian (that is, bilinear in Fermi fields) will lead to a free energy functional involving a trace such as that in equation (4.1). This is the result of integrating the fermions out of the problem. Consequently, many of the results in this work will generalize to some of these other systems. The principal difference may be the differing space dimensionality and order parameter structure; however, our investigations on vortices in type II superconductors [6] indicate that a representation of the free energy exists that has very great similarities to equation (4.1). In the recent numerical work of Gygi *et al* [7] on the low-temperature structure of vortices in extreme type II superconductors, the authors attribute the very large derivative of the order parameter at the vortex origin to bound states of electrons trapped on the vortex. The present work indicates the sensitivity of the bound state contribution in a related system to the derivative of the soliton profile, $|\Phi'(0)|$, and there is clearly a relation between these two findings. We hope to pursue this topic elsewhere.

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Appendix 1. Expansion of the function $\chi(\lambda)$

In this appendix we expand the function $\chi(\lambda)$, given in equation (3.8*b*), for large λ. We have

$$\chi(\lambda)=\frac{2}{\pi}\int_0^\infty \mathrm{d}t\,K_1(t)\frac{4\sinh^2(t/2)}{t}\left(\frac{1}{\mathrm{e}^{t/\lambda}-1}-\frac{\lambda}{t}+\frac{1}{2}\right). \tag{A1.1}$$

For large t we have

$$K_1(t)\frac{4\sinh^2(t/2)}{t}\sim\sqrt{\frac{\pi}{2}}\,t^{-3/2}. \tag{A1.2}$$

Let us write

$$\chi(\lambda)=\chi_1(\lambda)+\chi_2(\lambda) \tag{A1.3a}$$

$$\chi_1(\lambda)=\frac{2}{\pi}\int_0^\infty \mathrm{d}t\,\sqrt{\frac{\pi}{2}}\,t^{-3/2}\left(\frac{1}{\mathrm{e}^{t/\lambda}-1}-\frac{\lambda}{t}+\frac{1}{2}\right) \tag{A1.3b}$$

$$\chi_2(\lambda)=\frac{2}{\pi}\int_0^\infty \mathrm{d}t\left(K_1(t)\frac{4\sinh^2(t/2)}{t}-\sqrt{\frac{\pi}{2}}\,t^{-3/2}\right)\left(\frac{1}{\mathrm{e}^{t/\lambda}-1}-\frac{\lambda}{t}+\frac{1}{2}\right). \tag{A1.3c}$$

The change of variables $t=\lambda u$ makes manifest the λ dependence of $\chi_1(\lambda)$. The integral may be evaluated by expressing $1/(\mathrm{e}^u-1)$ in terms of $\coth(u/2)$ and then using the partial fraction decomposition. This leads to the following result for $\chi_1(\lambda)$:

$$\chi_1(\lambda)=\frac{\zeta(\frac{3}{2})}{\sqrt{2}\pi}\frac{1}{\sqrt{\lambda}}. \tag{A1.4}$$

Note that for $\chi_2(\lambda)$ the quantity

$$K_1(t)\frac{4\sinh^2(t/2)}{t}-\sqrt{\frac{\pi}{2}}\,t^{-3/2}$$

behaves for large t as $t^{-5/2}$. Thus, to obtain the correct behaviour up to and including $\mathrm{O}(\lambda^{-1})$ we can simply expand the second parentheses in the integrand of equation (A1.3*c*). This indicates that χ_2 has a large-λ expansion that begins at $\mathrm{O}(\lambda^{-1})$. It also indicates that χ_2 will not be analytic in λ^{-1} at higher order due to divergence of the coefficients, and additional considerations need to be given to extract these higher terms. Thus

$$\chi_2(\lambda) = O(\lambda^{-1}) \tag{A1.5}$$

and we obtain

$$\chi(\lambda) = \frac{\zeta(\frac{3}{2})}{\sqrt{2}\pi} \frac{1}{\sqrt{\lambda}} + O(\lambda^{-1}). \tag{A1.6}$$

Appendix 2. Proof of $\mathrm{Tr}\, f(x,p) = \mathrm{tr} \int \mathrm{d}k\, \mathrm{d}x\, f(x, k - \mathrm{i}\partial_x)/2\pi$

In this appendix we prove the relation between the quantum mechanical trace and the phase space integral.

The proof proceeds as follows. Consider a function f which depends on the coordinate and momentum operators x and p and also has unspecified matrix structure. On suppressing the matrix indices, we have

$$\begin{aligned}\langle x'|f(x,p)|x''\rangle &= f\left(x', -\mathrm{i}\frac{\partial}{\partial x'}\right)\langle x'|x''\rangle \\ &\equiv f(x', -\mathrm{i}\partial_{x'}) \int \frac{\mathrm{d}k}{2\pi} \mathrm{e}^{\mathrm{i}k(x'-x'')} \\ &= \int \frac{\mathrm{d}k}{2\pi} \mathrm{e}^{\mathrm{i}k(x'-x'')} f(x', k - \mathrm{i}\partial_{x'}).\end{aligned} \tag{A2.1}$$

Then, with tr denoting the matrix trace,

$$\mathrm{Tr}\, f(x,p) = \mathrm{tr} \int \mathrm{d}x' \langle x'|f(x,p)|x'\rangle \tag{A2.2}$$

and using equation (A2.1) with $x'' = x'$, we obtain the required result:

$$\mathrm{Tr}\, f(x,p) = \mathrm{tr} \int \frac{\mathrm{d}k\, \mathrm{d}x}{2\pi} f(x, k - \mathrm{i}\partial_x). \tag{A2.3}$$

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