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Non-analytic behaviour of the free energy of fermions coupled to small solitons

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Abstract. The free energy of condensed matter systems containing fermions coupled to small topological solitons is investigated. The exactly soluble continuum model of polyacetylene, with a hyperbolic tangent soliton profile, is shown to yield non-analytic terms in the free energy of the form $\lambda^n \ln \lambda$ where λ is a parameter proportional to the size of the soliton. A representation of the free energy that is suitable for a small λ-expansion is derived for general soliton profiles. The non-analytic expansion of the free energy about $\lambda = 0$ is found for a general soliton profile for the case of zero temperature.

1. Introduction

A number of different condensed matter systems that contain fermions also have the ability to support topological solitons. Examples that come to mind (the list is not exhaustive) are polyacetylene, type II superconductors and superfluid ^{3}He. In polyacetylene it is the dimerization which can interpolate between degenerate ground states, thereby forming a topological soliton. In the Fermi superfluids there can be vortices or domain walls in the order parameter and these may also be described as solitons. The objective we ultimately have in mind is to understand the low-temperature structure of vortices of type II superconductors. There have been conflicting claims made on whether the vortex core shrinks to effectively zero size at zero temperature [1] or whether the core remains finite [2]. It seems clear that a necessary step in the understanding of this problem is to be able to accurately calculate the free energy of such systems when the soliton size becomes small. The vortex possess cylindrical symmetry and thus has a two-dimensional character. It has additional complexity in that it is not just a coupled fermion–soliton problem since the vortex also has a magnetic field associated with it and it may be that a full treatment including consideration of the magnetic field is necessary.

The present paper deals with the simpler one-dimensional problem of calculating the free energy of small-size solitons in polyacetylene where only fermions and a soliton are present. This is a system for which the free energy is known for all soliton scales when the soliton is assumed to have a hyperbolic tangent (tanh) profile [3]. In section 2 we obtain the free energy for small-size solitons from the integral representation of the exact result for the tanh profile. In section 3 a general expression for the free energy is derived and in section 4 we evaluate this in the zero-size (sharp soliton) limit. Section 5 is concerned with extracting the corrections to the free energy for soliton profiles with a small but finite width and comparisons are made with the exact results. Section 6 discusses some aspects of the work and is followed by four appendices.

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2. Exact results for the tanh profile

In an earlier paper the free energy of polyacetylene was obtained for the case where the soliton profile had a hyperbolic tangent form [3]. With Δ_0 denoting the equilibrium dimerization of a uniform system the soliton was written as

$$\Delta(x)=\Delta_0 \tanh\left(\frac{x\Delta_0}{\lambda v_F}\right) \tag{2.1}$$

where v_F is the Fermi velocity and λ is a dimensionless parameter that characterizes the size of the soliton.

Explicit results for the zero-temperature limit of the free energy associated with the soliton (this quantity is denoted by $E-E_0$) is derived in [3] and in this section we shall extract the small λ-behaviour of this quantity. A convenient starting point is equation (D.6) of [3] which we rewrite in the slightly different form (K_0 denotes the Bessel function of imaginary argument with order zero [4])

$$\frac{E-E_0}{\Delta_0}=-1+\frac{2}{\pi}\int_0^\infty \mathrm{d}t\, K_0(t)\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\mathrm{e}^t+\mathrm{e}^{-t}-2}{t(1-\mathrm{e}^{-t/\lambda})}-\lambda\right). \tag{2.2}$$

This may be now integrated by parts and rearranged to yield

$$\begin{aligned}\frac{E-E_0}{\Delta_0}=&-1+\frac{2}{\pi}\int_0^\infty \mathrm{d}t\, K_1(t)\frac{(\mathrm{e}^t+\mathrm{e}^{-t}-2)}{t}\\&+\frac{2}{\pi}\int_0^\infty \mathrm{d}t\, K_1(t)\left[\frac{\mathrm{e}^t+\mathrm{e}^{-t}-2}{t}\left(\frac{1}{1-\mathrm{e}^{-t/\lambda}}-1\right)-\lambda\right].\end{aligned} \tag{2.3}$$

Using the integral representation of the Bessel function [4]

$$K_1(t)=t\int_1^\infty \mathrm{d}u(u^2-1)^{1/2}\,\mathrm{e}^{-ut} \tag{2.4}$$

it quickly follows that the first two terms in equation (2.3) add to yield unity, and thus we can write

$$\frac{E-E_0}{\Delta_0}=1+\frac{2}{\pi}\Psi(\lambda) \tag{2.5}$$

where

$$\Psi(\lambda)=\int_0^\infty \mathrm{d}t\, K_1(t)\left(\frac{4\sinh^2(t/2)}{t}\,\frac{1}{\mathrm{e}^{t/\lambda}-1}-\lambda\right). \tag{2.6}$$

In appendix 1 the behaviour of $\Psi(\lambda)$ for small λ is derived. An interesting non-analytic behaviour involving logarithms is found. Up to and including terms of order $\lambda^3\ln\lambda$ and λ^3 the function $\Psi(\lambda)$ has the form

$$\Psi(\lambda)=(a_1\lambda+a_3\lambda^3+\ldots)\ln\lambda+(b_1\lambda+b_3\lambda^3+\ldots) \tag{2.7a}$$

$$a_1=1 \tag{2.7b}$$

$$a_3=\zeta(3) \tag{2.7c}$$

$$b_1=\gamma-\ln 2 \tag{2.7d}$$

$$b_3=(\tfrac{7}{6}-\ln 2)\zeta(3)+\zeta'(3) \tag{2.7e}$$

(here and elsewhere in the paper, $'$ denotes differentiation with respect to the argument of any function). In the following sections we shall provide a method to extract the leading terms in the small-λ expansion of the soliton creation energy for general soliton profiles. Note in particular that at precisely $\lambda = 0$ we have $\Psi(0) = 0$ and thus

$$\left.\frac{(E - E_0)}{\Delta_0}\right|_{\lambda=0} = 1. \tag{2.8}$$

3. General expression for the free energy

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 $\Delta(x)$ [5]. 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 obtained from the ratio of two functional determinants (more details of this can be found in section 2 of [3]). Let ψ and $\bar{\psi}$ be independent Grassmann fields which are functions of the Euclidean time variable τ and are antiperiodic in τ over the interval β ($\equiv$inverse temperature). Then we can write

$$\exp[-\beta(F - F_0)] = \frac{\int \mathrm{d}\bar{\psi}\, \mathrm{d}\psi \exp(-\int_0^\beta \mathrm{d}\tau \int \mathrm{d}x\, \bar{\psi}(\partial_\tau + H)\psi)}{\int \mathrm{d}\bar{\psi}\, \mathrm{d}\psi \exp(-\int_0^\beta \mathrm{d}\tau \int \mathrm{d}x\, \bar{\psi}(\partial_\tau + H_0)\psi)} \exp(-\beta\Omega \int \mathrm{d}x(\Delta^2 - \Delta_0^2)) \tag{3.1a}$$

where

$$H = -\mathrm{i}v_\mathrm{F}\partial_x\sigma_3 + \Delta(x)\sigma_1 \tag{3.1b}$$

$$H_0 = -\mathrm{i}v_\mathrm{F}\partial_x\sigma_3 + \Delta_0\sigma_1 \tag{3.1c}$$

Ω is a combination of spring and coupling constants (that need not concern us here) and σ_k ($k = 1, 2, 3$) are the Pauli matrices. They describe the physics of electrons moving at $\pm v_\mathrm{F}$; they are not connected with spin which 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

$$F - F_0 = -\frac{2}{\beta}\ln\left(\frac{\mathrm{Det}(\partial_\tau + H)}{\mathrm{Det}(\partial_\tau + H_0)}\right) + \Omega \int \mathrm{d}x(\Delta^2 - \Delta_0^2) \tag{3.2}$$

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_n and $-\omega_m$ (with a requisite factor of $\frac{1}{2}$ in front of the logarithm; this point is discussed in appendix A of [3]). The result is (det denotes the determinant taken over reduced space where the eigenfunctions depend only on x and Pauli indices)

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

Next we introduce the Green function

$$G_0(\omega_m) = \frac{1}{\omega_m^2 + H_0^2} \equiv \frac{1}{\omega_m^2 + v_\mathrm{F}^2 p^2 + \Delta_0^2} \tag{3.4}$$

which we regard as an operator in which the states are labelled by spatial coordinates as well as by the suppressed Pauli indices:

$$\langle x|G_0(\omega_m)|x'\rangle = G_0(x, x'; \omega_m). \tag{3.5}$$

Finally to obtain the desired form for $F - F_0$ we (i) use the identity

$$\ln \det \equiv \mathrm{Tr} \ln \tag{3.6}$$

where Tr denotes the trace taken over the reduced space noted above (with only spatial and matrix degrees of freedom) and (ii) employ the alternative representation of the dimerization contribution appearing in equation (3.1a):

$$\Omega \int \mathrm{d}x(\Delta^2 - \Delta_0^2) = \frac{1}{\beta}\sum_m \mathrm{Tr}\, G_0(\omega_m)(H^2 - H_0^2). \tag{3.7}$$

This equation follows from stationarity of the free energy F_0 of a uniformly dimerized system with respect to variations of Δ_0 and is derived in appendix 2. It straightforwardly follows that

$$F - F_0 = -\frac{1}{\beta}\sum_m \{\mathrm{Tr} \ln[1 + G_0(\omega_m)(H^2 - H_0^2)] - \mathrm{Tr}[G_0(\omega_m)(H^2 - H_0^2)]\} \tag{3.8}$$

and this is an expression we shall make use of in the remainder of this work.

4. Evaluating the free energy in the sharp solution ($\lambda = 0$) limit

The form of the free energy given in equation (3.8) rather naturally suggests the expansion of the logarithm in powers of $G_0(H^2 - H_0^2)$:

$$F - F_0 = \frac{1}{\beta}\sum_m \sum_{n=2}^{\infty} \frac{(-1)^n}{n} \mathrm{Tr}\{[G_0(\omega_m)(H^2 - H_0^2)]^n\} \tag{4.1}$$

(the question of convergence of such a series has been addressed in [6]). It follows from equation (3.1b) and (3.1c) that

$$H^2(x) - H_0^2(x) = \Delta^2(x) - \Delta_0^2 + \sigma_2 v_F \Delta'(x). \tag{4.2}$$

For present and future use let us consider a general soliton profile (which therefore includes the tanh as a special case) and write

$$\Delta(x) = \Delta_0 \Phi\left(\frac{x\Delta_0}{\lambda v_F}\right) \tag{4.3}$$

where the profile Φ is an odd, monotonically increasing function that approaches ± 1 at spatial infinity:

$$\Phi(\pm\infty) = \pm 1. \tag{4.4}$$

We shall assume in what follows that the typical scale of variation of Φ is of order unity, i.e. $\Phi'(0) \sim 1$ and that λ is the appropriate dimensionless measure of the soliton size. In terms of Φ, we have

$$H^2(x) - H_0^2(x) = \Delta_0^2 \Phi^2\left(\frac{x\Delta_0}{\lambda v_F}\right) - \Delta_0^2 + \sigma_2 \frac{\Delta_0^2}{\lambda} \Phi'\left(\frac{x\Delta_0}{\lambda v_F}\right). \tag{4.5}$$

The limit that is required of this quantity in the present section is $\lambda \to 0$ since this yields a sharp soliton of vanishing size in which the dimerization discontinuously jumps from $-\Delta_0$ to $+\Delta_0$. Despite the apparently singular form of $(H^2 - H_0^2)$ in this limit the series in equation (4.1) for the free energy can be summed to yield a finite result, as we shall now show.

The soliton free energy is

$$\begin{aligned}\frac{1}{\beta}\sum_m \sum_{n=2}^{\infty} &\frac{(-1)^n}{n} \operatorname{Tr}\{[G_0(\omega_m)(H^2 - H_0^2)]^n\} \\ &= \frac{1}{\beta}\sum_m \sum_{n=2}^{\infty} \frac{(-1)^n}{n} \operatorname{tr} \int \mathrm{d}x_1 \ldots \mathrm{d}x_n \langle x_1|G_0(\omega_m)|x_2\rangle \ldots \langle x_n|G_0(\omega_m)|x_1\rangle \\ &\quad \times (H^2(x_1) - H_0^2(x_1)) \ldots (H^2(x_n) - H_0^2(x_n))\end{aligned} \tag{4.6}$$

where tr denotes the trace over matrix indices. The matrix element of the Green's function is

$$\begin{aligned}\langle x_1|G_0(\omega_m)|x_2\rangle &= \int \frac{\mathrm{d}p}{2\pi} \exp[\mathrm{i}p(x_1 - x_2)] \frac{1}{\omega_m^2 + v_F^2 p^2 + \Delta_0^2} \\ &= \frac{1}{2\Delta_0 v_F} \frac{\exp[-(\Delta_0/v_F)|x_1 - x_2|\sqrt{1+\nu_m^2}]}{\sqrt{1+\nu_m^2}}\end{aligned} \tag{4.7}$$

where we have defined

$$\nu_m = \omega_m / \Delta_0. \tag{4.8}$$

Let us now define new integration variables y_i defined by

$$y_i = \frac{x_i \Delta_0}{\lambda v_F} \qquad i = 1, 2, \ldots, n \tag{4.9}$$

and a scaled version of the 'interaction' $H^2 - H_0^2$,

$$f_\sigma(y; \lambda) = \sigma \Phi'(y) - \lambda(1 - \Phi^2(y)) \tag{4.10}$$

where $\sigma (= \pm 1)$ are the eigenvalues of σ_2. We can then write

$$\begin{aligned}(F - F_0) = \frac{1}{\beta}\sum_m \sum_\sigma \sum_{n=2}^{\infty} &\frac{(-1)^n}{2^n n} \frac{1}{(1+\nu_m^2)^{n/2}} \int \mathrm{d}y_1 \ldots \mathrm{d}y_n \\ &\times \exp[-\lambda\sqrt{1+\nu_m^2}(|y_1 - y_2| + \ldots |y_n - y_1|)] f_\sigma(y_1; \lambda) \ldots f_\sigma(y_n; \lambda).\end{aligned} \tag{4.11}$$

The soliton free energy in the limit $\lambda \to 0$ may be obtained by setting $\lambda = 0$ in this equation (we assume $\int \mathrm{d}y(1 - \Phi^2(y))$ is finite) with the result

$$\begin{aligned}F - F_0 &= \frac{1}{\beta}\sum_m \sum_\sigma \sum_{n=2}^{\infty} \frac{(-1)^n}{n} \frac{1}{(1+\nu_m^2)^{n/2}} \left(\sigma \cdot \tfrac{1}{2} \int \mathrm{d}y\, \Phi'(y)\right)^n \\ &= -\frac{1}{\beta}\sum_m \ln\left(\frac{\nu_m^2}{1+\nu_m^2}\right).\end{aligned} \tag{4.12}$$

Note that in the $\lambda = 0$ limit the free energy is entirely determined by the topology of the soliton since only the 'topological winding number' $\frac{1}{2}\int \mathrm{d}y\, \Phi'(y)$ (=+1 for solitons and -1 for antisolitons) appears in the result.

It is straightforward to specialize the result to zero temperature with the answer

$$\lim_{T\to 0}(F-F_0)/\Delta_0|_{\lambda=0} \equiv (E-E_0)/\Delta_0|_{\lambda=0}=1 \tag{4.13}$$

in agreement with the exact result.

5. Leading corrections to the free energy due to finite soliton size

Once equation (4.11) for the free energy is obtained it is possible to generate the leading corrections to the $\lambda=0$, sharp soliton, limit. Here we shall indicate how to derive the corrections to the soliton free energy that are of order $\lambda \ln \lambda$ and λ (higher-order terms are of the form $\lambda^n \ln \lambda$ and λ^n with $n>1$). Our calculations will be restricted to the case of zero temperature (and thus sums over frequencies are replaced by integrals). Higher-order corrections and finite-temperature effects may be obtained by the appropriate generalization of the considerations given below.

To proceed we look at three different contributions to the zero temperature limit of the soliton free energy, which, in units of Δ_0, is $(E-E_0)/\Delta_0$.

(a) Some terms of order λ follow from the dependence of $f_\sigma(y;\lambda)$ on λ. The contribution is

$$\begin{aligned}
I_a &= \int_0^\infty \frac{\mathrm{d}\nu}{\pi}\sum_{n=2}^{\infty}\sum_\sigma \frac{(-1)^n}{2^n n}\frac{1}{(1+\nu^2)^{n/2}}\, n \\
&\quad\times \int \mathrm{d}y_1\ldots\mathrm{d}y_n[-\lambda(1-\Phi^2(y_1)]f_\sigma(y_2;0)\ldots f_\sigma(y_n;0) \\
&= -\frac{\lambda}{2}\int_0^\infty \frac{\mathrm{d}\nu}{\pi}\sum_{n=2}^{\infty}\sum_\sigma (-1)^n\frac{1}{(1+\nu^2)^{n/2}}\int \mathrm{d}y_1(1-\Phi^2(y_1))\left(\sigma\cdot\tfrac{1}{2}\int \Phi'(y)\,\mathrm{d}y\right)^{n-1} \\
&= \lambda\int_0^\infty \frac{\mathrm{d}\nu}{\pi}\sum_{n=1}^{\infty}\frac{1}{(1+\nu^2)^{n+1/2}}\int \mathrm{d}y(1-\Phi^2(y)).
\end{aligned} \tag{5.1}$$

(b) Another source of terms of order λ arises from the linear term in the expansion of the exponential combined with terms with $n\geqslant 3$ from the sum over n. This yields

$$\begin{aligned}
I_b &= -\lambda\int_0^\infty \frac{\mathrm{d}\nu}{\pi}\sum_{n=3}^{\infty}\sum_\sigma \frac{(-1)^n}{2^n n}\frac{1}{(1+\nu^2)^{(n-1)/2}} \\
&\quad\times\int \mathrm{d}y_1\ldots\mathrm{d}y_n(|y_1-y_2|+\ldots|y_n-y_1|)f_\sigma(y_1;0)\ldots f_\sigma(y_n;0) \\
&= -\frac{\lambda}{4}\int_0^\infty \frac{\mathrm{d}\nu}{\pi}\sum_{n=3}^{\infty}\sum_\sigma \frac{(-1)^n}{n}\frac{1}{(1+\nu^2)^{(n-1)/2}}\, n \\
&\quad\times\int \mathrm{d}y_1\,\mathrm{d}y_2|y_1-y_2|\Phi'(y_1)\Phi'(y_2)\left(\sigma\cdot\tfrac{1}{2}\int \mathrm{d}y\,\Phi'(y)\right)^{n-2} \\
&= -\lambda\int_0^\infty \frac{\mathrm{d}\nu}{\pi}\sum_{n=1}^{\infty}\frac{1}{(1+\nu^2)^{n+1/2}}\frac{1}{2}\int \mathrm{d}y_1\,\mathrm{d}y_2|y_1-y_2|\Phi'(y_1)\Phi'(y_2).
\end{aligned} \tag{5.2}$$

(c) Contributions of order λ and $\lambda \ln \lambda$ arise from the term in the sum over n with $n=2$. The expansion of the exponential used in (b) would, formally, yield an infinite result if it were carried out on the term with $n=2$, indicating the incorrectness of this step. What is required is a more careful treatment of this term. The contribution that is independent of terms already counted in I_a and the $\lambda=0$ result is given by

$$I_c=\int_0^\infty \frac{d\nu}{\pi}\sum_\sigma \frac{1}{8(1+\nu^2)}\int dy_1\, dy_2(\exp(-2\lambda\sqrt{1+\nu^2}|y_1-y_2|)-1)f_\sigma(y_1;0)f_\sigma(y_2;0)$$

$$=\int_0^\infty \frac{d\nu}{1+\nu^2}\int dy_1\, dy_2(\exp(-2\lambda\sqrt{1+\nu^2}|y_1-y_2|)-1)\Phi'(y_1)\Phi'(y_2). \tag{5.3}$$

The frequency integral that appears in equation (5.3) is of the form $\int_0^\infty d\nu(1+\nu^2)^{-1}$ $[\exp(-\alpha\sqrt{1+\nu^2})-1]$. In appendix 3 this is expanded up to order $\alpha \ln \alpha$ and α. The result is

$$\int_0^\infty d\nu(1+\nu^2)^{-1}[\exp(-\alpha\sqrt{1+\nu^2})-1]=\alpha \ln \alpha-\alpha(1-\gamma+\ln 2)+\ldots. \tag{5.4}$$

and thus to terms of order $\lambda \ln \lambda$ and λ

$$I_c=\lambda \ln \lambda \int \frac{dy_1\, dy_2}{2\pi}|y_1-y_2|\Phi'(y_1)\Phi'(y_2)$$

$$+\lambda\int dy_1\, dy_2[|y_1-y_2|\ln|y_1-y_2|-(1-\gamma)|y_1-y_2|]\Phi'(y_1)\Phi'(y_2). \tag{5.5}$$

There are no further terms of order λ or $\lambda \ln \lambda$ in $F-F_0$ and all that remains is to combine I_a, I_b and I_c in a convenient form.

Ultimately, all λ dependence in the problem arises from the original choice, equation (4.3), for the soliton form, however the contributions of I_a and I_b to the free energy do seem to have quite distinct origins; I_a arising from the 'interaction' and I_b from the behaviour of the Green's function. It should be noted that individually I_a and I_b diverge on integration over ν. To obtain a finite result there must be a substantial cancellation between these two terms. It turns out that by virtue of the identity (a proof of which may be found in appendix 4)

$$\int dy(1-\Phi^2(y))\equiv\tfrac{1}{2}\int dy_1\, dy_2|y_1-y_2|\Phi'(y_1)\Phi'(y_2) \tag{5.6}$$

I_a and I_b precisely cancel with each other (this cancellation also holds, unchanged, at finite temperatures). We can therefore combine the $\lambda=0$ result with the contribution of I_c to write the soliton creation energy for general soliton profiles as

$$\frac{E-E_0}{\Delta_0}=1+\frac{2}{\pi}(a_1\lambda \ln \lambda+b_1\lambda+\ldots) \tag{5.7a}$$

$$a_1=\tfrac{1}{4}\int dy_1\, dy_2|y_1-y_2|\Phi'(y_1)\Phi'(y_2) \tag{5.7b}$$

$$b_1=\tfrac{1}{4}\int dy_1\, dy_2[|y_1-y_2|\ln|y_1-y_2|-(1-\gamma)|y_1-y_2|]\Phi'(y_1)\Phi'(y_2). \tag{5.7c}$$

It may be verified that on choosing the soliton profile $\Phi(y)$ to be $\tanh(y)$ that the results for a_1 and b_1 given above agree with those given in equations (2.7*b*) and (2.7*d*).

6. Discussion

In this work we have shown that by going to an appropriate representation of the soliton free energy, namely equation (4.11), it is possible to evaluate corrections to the sharp soliton limit arising from the finite extent of the soliton. We have seen that terms logarithmic in λ arise from the detailed spatial behaviour of the Green's function G_0. From the way the $\lambda \ln \lambda$ term originated it is possible to understand where higher-order terms of order $\lambda^s \ln \lambda$ come from. In essence this is from the expansion of frequency integrals of the form $\int_0^\infty \mathrm{d}\nu(1+\nu^2)^{-n/2} \exp(-\lambda\sqrt{1+\nu^2}r)$ that appear in the (zero-temperature limit of the) free energy. For large ν the integral is approximately $\int^\infty \mathrm{d}\nu\, \nu^{-n} \exp(-\lambda\nu r)$ and it is intuitively obvious that we can correctly generate terms in λ up to and including λ^{n-2} by simply expanding the exponential. The term in λ^{n-1} derived in this way has a coefficient which diverges logarithmically and this suggests that there will be terms of order $\lambda^{n-1} \ln \lambda$ present in the expansion of the integral (along with λ^{n-1} and higher-order terms). An appropriate treatment of the integrals indicates that these intuitive considerations are correct. It follows that the term in $\lambda^{s-1} \ln \lambda$ in the free energy arises from all terms in the sum over n with $n \leqslant s$. Thus, for a small value of s a relatively small amount of work is needed to determine the term in $\lambda^{s-1} \ln \lambda$. This is in contrast to the term in λ^{s-1} which appears to require a careful combinatoric analysis to determine its contribution.

An inspection of the exact results for the expansion of the free energy (equations (2.5), (2.6) and (2.7)) appears to indicate that when $\lambda^s \ln \lambda$ is present then so is λ^s and that only odd values of s appear. For the exact results this seems to be a feature inherited from the property of the Bessel function that appears in the integrand (although we have not proved it for general s). A significant efficiency of calculation would be achieved if we could see, from some general considerations of the free energy given in equation (4.1), why (if true) (i) only odd powers of λ appear and (ii) how to infer the coefficient of λ^s from knowledge of the coefficient of $\lambda^s \ln \lambda$? We do not know how to answer either of these questions and leave them as open problems.

As stated in the introduction, this work is a preliminary step in the understanding of solitons (vortices) that may, genuinely, be small at low temperatures. This is in contrast to the solitons of the system studied in this work, whose equilibrium size and creation energy are given by [3]

$$\lambda = 1 \qquad (E - E_0)/\Delta_0 = 2/\pi \approx 0.6366 \qquad \text{Exact.} \tag{6.1}$$

It is nevertheless interesting to see just how close these values can be reached by the small-λ results given in this work. Using the exact results of equations (2.5), (2.6) and (2.7) we can determine the value of λ that minimizes $(E - E_0)/\Delta_0$ for the lowest-order 'linear' calculation where only $\lambda \ln \lambda$ and λ are included and the next-order 'cubic' calculation where terms up to $\lambda^3 \ln \lambda$ and λ^3 are included. We find that at the minimum

$$\lambda = 0.413 \qquad (E - E_0)/\Delta_0 = 0.737 \qquad \text{linear} \tag{6.2}$$

$$\lambda = 0.456 \qquad (E - E_0)/\Delta_0 = 0.704 \qquad \text{cubic.} \tag{6.3}$$

These are remarkably close to the exact results given the low order of the terms kept. They suggest that if very small solitons were energetically favoured, considerable confidence could be had in the predictions of a small-λ expansion which was truncated at low order.

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Appendix 1. Behaviour of $\Psi(\lambda)$ for small λ

In this appendix we shall derive the leading behaviour of the function

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

for values of $\lambda \ll 1$.

We split the range of integration into two parts, $t\leqslant\alpha\lambda$ and $t\geqslant\alpha\lambda$, where we consider α arbitrary but of order unity. For the integral with $t\leqslant\alpha\lambda$, which we denote by $\Psi_1(\lambda)$, we use the identities

$$\lambda\frac{\mathrm{d}}{\mathrm{d}t}\ln(1-\mathrm{e}^{-t/\lambda})\equiv\frac{1}{\mathrm{e}^{t/\lambda}-1} \tag{A1.2}$$

$$\lambda\frac{\mathrm{d}}{\mathrm{d}t}\ln\left(\frac{t}{\lambda}\right)\equiv\frac{\lambda}{t} \tag{A1.3}$$

to integrate by parts with the result

$$\Psi_1(\lambda)=\lambda\alpha\lambda K_1(\alpha\lambda)\left(\frac{4\sinh^2(\alpha\lambda/2)}{(\alpha\lambda)^2}\ln(1-\mathrm{e}^{-\alpha})-\ln\alpha\right)$$
$$-\lambda\int_0^{\alpha\lambda}\mathrm{d}t\left[\ln(1-\mathrm{e}^{-t/\lambda})\frac{\mathrm{d}}{\mathrm{d}t}\left(tK_1(t)\frac{4\sinh^2(t/2)}{t^2}\right)-\ln\left(\frac{t}{\lambda}\right)\frac{\mathrm{d}}{\mathrm{d}t}(tK_1(t))\right]. \tag{A1.4}$$

Within the integrals we make the small-t expansions [4]

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(tK_1(t)\frac{4\sinh^2(t/2)}{t^2}\right)=t\ln t+at+\ldots \tag{A1.5a}$$

$$a=\tfrac{1}{6}+\gamma-\ln 2 \tag{A1.5b}$$

(γ is Euler's constant),

$$\frac{\mathrm{d}}{\mathrm{d}t}[tK_1(t)]=t\ln t+bt+\ldots \tag{A1.6a}$$

$$b=\gamma-\ln 2 \tag{A1.6b}$$

and change variable from t to u with

$$t=\lambda u \tag{A1.7}$$

with the result

$$\Psi_1(\lambda)=\lambda\alpha\lambda K_1(\alpha\lambda)\left(\frac{4\sinh^2(\alpha\lambda/2)}{(\alpha\lambda)^2}\ln(1-\mathrm{e}^{-\alpha})-\ln\alpha\right)$$
$$-\lambda^3\ln\lambda\int_0^\alpha \mathrm{d}u[u\ln(1-\mathrm{e}^{-u})-u\ln u]$$
$$-\lambda^3\int_0^\alpha \mathrm{d}u[(u\ln u+au)\ln(1-\mathrm{e}^{-u})-(u\ln u+bu)\ln u]+\ldots. \tag{A1.8}$$

For the integral with $t \geqslant \alpha\lambda$, which we denote by $\Psi_2(\lambda)$, we employ again the identity equation (A1.2), integrate by parts and also use $K_1(t) = -K_0'(t)$ [4] to obtain

$$\Psi_2(\lambda) = -\lambda\alpha\lambda K_1(\alpha\lambda)\frac{4\sinh^2(\alpha\lambda/2)}{(\alpha\lambda)^2}\ln(1-e^{-\alpha})$$

$$-\lambda\int_{\alpha\lambda}^{\infty} dt \ln(1-e^{-t/\lambda})\frac{d}{dt}tK_1(t)\frac{4\sinh^2(t/2)}{t^2} - \lambda K_0(\alpha\lambda). \qquad \text{(A1.9)}$$

Since the integral gets its principal contribution from small t we use the expansion of equation (A1.5) and, on changing variables to u, equation (A1.7), we obtain

$$\Psi_2(\lambda) = -\lambda\alpha\lambda K_1(\alpha\lambda)\frac{4\sinh^2(\alpha\lambda/2)}{(\alpha\lambda)^2}\ln(1-e^{-\alpha}) - \lambda^3\ln\lambda\int_{\alpha}^{\infty} du\, u\ln(1-e^{-u})$$

$$-\lambda^3\int_{\alpha}^{\infty} du\,(u\ln u + au)\ln(1-e^{-u}) - \lambda K_0(\alpha\lambda) + \ldots. \qquad \text{(A1.10)}$$

Finally, we combine Ψ_1 and Ψ_2 from equations (A1.8) and (A1.10) and expand the combination $\alpha\lambda K_1(\alpha\lambda)\ln\alpha + K_0(\alpha\lambda)$ up to order $\lambda^2\ln\lambda$, λ^2 [4]. We find a result that is, to the order we are working at, independent of α (as it must be) and is given by

$$\Psi(\lambda) = (a_1\lambda + a_3\lambda^3 + \ldots)\ln\lambda + (b_1\lambda + b_3\lambda^3 + \ldots) \qquad \text{(A1.11}a\text{)}$$

$$a_1 = 1 \qquad \text{(A1.11}b\text{)}$$

$$a_3 = -\int_0^{\infty} du\, u\ln(1-e^{-u}) = \zeta(3) \qquad \text{(A1.11}c\text{)}$$

$$b_1 = \gamma - \ln 2 \qquad \text{(A1.11}d\text{)}$$

$$b_3 = -\int_0^{\infty} du[u\ln u + (\tfrac{1}{6} + \gamma - \ln 2)u]\ln(1-e^{-u})$$

$$= (\tfrac{7}{6} - \ln 2)\zeta(3) + \zeta'(3). \qquad \text{(A1.11}e\text{)}$$

Appendix 2. An alternative form of the dimerization term that follows from stationarity of the free energy of a uniform system, F_0, with respect to Δ_0

In this appendix we rewrite the dimerization term (the final term in equation (3.1a)). We use the fact the the dimerization of a uniform system is determined by requiring that the free energy is stationary (a minimum) with respect to variations of Δ_0. This amounts to the requirement that

$$\frac{\partial}{\partial\Delta_0^2}\left(-\frac{1}{\beta}\sum_m \mathrm{Tr}\ln G_0^{-1}(\omega_m) + \Omega L\Delta_0^2\right) = 0 \qquad \text{(A2.1)}$$

where L is the length of the system. Thus

$$\frac{1}{\beta}\sum_m \mathrm{Tr}\, G_0(\omega_m) = \Omega L. \qquad \text{(A2.2)}$$

Since $\langle x|G_0(\omega_n)|x'\rangle$ is a function of $(x-x')$ we can write this equation for arbitrary x as (tr denotes the trace over matrix indices)

$$\frac{1}{\beta}\sum_m \mathrm{tr}\langle x|G_0(\omega_m)|x\rangle=\Omega. \tag{A2.3}$$

Let us consider now

$$\begin{aligned}\frac{1}{\beta}\sum_m \mathrm{Tr}\; G_0(\omega_m)(H^2-H_0^2) &= \frac{1}{\beta}\mathrm{tr}\sum_m \int \mathrm{d}x\langle x|G_0(\omega_m)|x\rangle(H^2(x)-H_0^2(x)) \\ &= \frac{1}{\beta}\int \mathrm{d}x\sum_m \mathrm{tr}(\langle x|G_0(\omega_m)|x\rangle)\tfrac{1}{2}\,\mathrm{tr}(H^2(x)-H_0^2(x))\end{aligned} \tag{A2.4}$$

where the last equation uses the fact that the Green's function is proportional to the unit matrix. By virtue of equation (A2.3) we can eliminate the sum involving the Green's function in favour of the 'coupling constant' Ω and obtain

$$\begin{aligned}\frac{1}{\beta}\sum_m \mathrm{Tr}\; G_0(\omega_m)(H^2-H_0^2) &= \Omega\tfrac{1}{2}\int \mathrm{d}x\; \mathrm{tr}(H^2(x)-H_0^2(x)) \\ &= \Omega\int \mathrm{d}x(\Delta^2(x)-\Delta_0^2)\end{aligned} \tag{A2.5}$$

which is the form used in the main text.

A point to note is that all of the terms in the expansion of the logarithm in powers of $G_0(H^2-H_0^2)$ in equation (4.1), only the term with $n=1$ (that cancels with the dimerization term) is in any way sensitive to the electronic bandwidth W. (We are assuming a weak-coupling theory where $\Delta_0/W \ll 1$.) As a consequence equation (A2.2) is the only place where momentum integrals have to be constrained and therefore the only important place the bandwidth enters the theory is in the uniform dimerization amplitude Δ_0.

Appendix 3. Small-α behaviour of the integral $\int_0^\infty \mathrm{d}\nu(1+\nu^2)^{-1}[\exp(-\alpha\sqrt{1+\nu^2})-1]$

In this appendix we derive the small-α behaviour of the above integral.

Writing

$$I(\alpha)=\int_0^\infty \mathrm{d}\nu(1+\nu^2)^{-1}[\exp(-\alpha\sqrt{1+\nu^2})-1] \tag{A3.1}$$

we note that

$$I(0)=0 \tag{A3.2}$$

$$I'(\alpha)=-\int_0^\infty \mathrm{d}\nu(1+\nu^2)^{-1/2}\exp(-\alpha\sqrt{1+\nu^2}). \tag{A3.3}$$

With the substitution $t=\sinh u$ it may be seen that $I'(\alpha)$ is, up to an overall sign difference, a Bessel function [4]:

$$I'(\alpha)=-K_0(\alpha). \tag{A3.4}$$

Thus, using equation (A3.2)

$$I(\alpha) = -\int_0^\alpha ds\, K_0(s). \tag{A3.5}$$

We can now use the small-s expansion of $K_0(s)$ [4]:

$$K_0(s) = -[\ln(s/2) + \gamma] + \ldots \tag{A3.6}$$

to find that up to terms of order $\alpha \ln \alpha$ and α

$$I(\alpha) = \alpha \ln \alpha - \alpha(1 - \gamma + \ln 2) + \ldots. \tag{A3.7}$$

Note that in the main text we identify

$$\alpha = 2\lambda |y_1 - y_2|. \tag{A3.8}$$

Since equation (A3.7) contains $\alpha \ln \alpha$, use of equation (A3.8) implies that this logarithmic term generates both $\lambda \ln \lambda$ and λ contributions. It thus seems that a consistent treatment which keeps terms of order $\lambda \ln \lambda$ should also keep terms linear in λ since they have, in part at least, common origins and this viewpoint has been taken throughout the paper.

Appendix 4. Proof of an identity

In this appendix we prove the identity

$$\int dy (1 - \Phi^2(y)) \equiv \tfrac{1}{2} \int dy_1\, dy_2 |y_1 - y_2| \Phi'(y_1)\Phi'(y_2) \tag{A4.1}$$

which holds for odd functions with

$$\Phi(\pm\infty) = \pm 1. \tag{A4.2}$$

The RHS of equation (A4.1) can be written as

$$I = I_1 + I_2 \tag{A4.2a}$$

with

$$I_1 = \int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{y_1} dy_2\, y_1 \Phi'(y_1)\Phi'(y_2) \tag{A4.2b}$$

and

$$I_2 = -\int_{-\infty}^{\infty} dy_1 \int_{-\infty}^{y_1} dy_2\, y_2 \Phi'(y_1)\Phi'(y_2). \tag{A4.2c}$$

For I_1 we integrate with respect to y_2 to obtain

$$I_1 = \int_{-\infty}^{\infty} dy_1\, y_1 \Phi'(y_1)(\Phi(y_1) - \Phi(-\infty)). \tag{A4.3}$$

Using oddness of Φ, we can omit the boundary term and write

$$I_1 = \int_{-\infty}^{\infty} dy_1\, y_1 \frac{d}{dy_1} \tfrac{1}{2}(\Phi^2(y_1) - 1). \tag{A4.4}$$

Integrating by parts shows that I_1 is precisely half the LHS of equation (A4.1). Similar manipulations on I_2 show that it is equal to I_1 and the identity is proved.

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