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Approximate calculation of the free energy of Fermi systems with topological solitons: soliton creation energy of polyacetylene

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Abstract. In this paper, we investigate an approximate technique for the calculation of the free energy of fermionic systems that are coupled to topological solitons. We apply this to a solvable one-dimensional model field theory: polyacetylene in the static dimerization approximation. We estimate the free energy of solitons with various scales of spatial extension and make comparisons with exact results. In an appendix, we make the connection between the high-temperature limit of our work and Ginzburg–Landau theory.

1. Introduction

In the many-body physics of fermions there are a number of cases where the second quantized Hamiltonian may be written as an operator that is bilinear in the fermion field operators. This happens, for example, in conventional singlet superconductors and in triplet Fermi superfluids where the interaction between the fermions results in a non-zero 'gap' (= order parameter) appearing. This results in the quartic interaction term being replaced by terms that are simultaneously bilinear in the fermionic field operators and linear in the order parameter. Another example, corresponding to quite a different situation, occurs in polyacetylene [1], where the coupling of electrons (assumed here to be non-interacting among themselves) and phonons (of wavenumber $2k_F$) leads to dynamic symmetry breaking in the phonon field. A non-zero order parameter results—the dimerization (the lattice undergoes a Peierls transition to a dimerized ground state). The dimerization order parameter couples to an operator bilinear in electron field operators.

While there are great similarities between the mathematical descriptions of the above systems (apart from, in general, differing space dimensionality), this does not necessarily imply that the physics is similar. Indeed, the field operators occurring in the superconductor/superfluid Hamiltonian act in Nambu (particle–hole and spin) space, while in polyacetylene the essential space is that of right- and left-moving electrons (travelling at the Fermi velocity).

In this paper, we present an approximation we have developed for the free energy—expressed solely in terms of the appropriate order parameter, and hence generalizing the Ginzburg–Landau free energy for $T \lesssim T_C$ (the transition temperature) to an arbitrary

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temperature. The method applies to systems involving fermions whose effective Hamiltonian is bilinear in field operators and whose order parameter possesses non-trivial spatial dependence (for example, topological solitons or vortices).

The approximation enables us to obtain quite reasonable estimates for the free energy over the full temperature range 0 to T_C. At temperatures close to T_C our results reduce to Ginzburg–Landau theory, as we show in appendix 2. At lower temperatures we find that it is very important to take into account the low-lying modes of the system. The most important of these are the bound states localized around the soliton, and any theory that omits consideration of these will make a very large error in the soliton creation energy.

In order to concentrate on the essential features of our approximation and not to be distracted by complications associated with space dimensionality or additonal degrees of freedom (e.g. electromagnetic fields) or dynamics of the order parameter, we shall focus our attention on polyacetylene in the static dimerization approximation. Thus the kinetic energy of the lattice is neglected from the free energy. We shall view this as the simplest one-dimensional system that can support solitons and thus serve as an interesting application of our methods (it is also sufficiently simple that effectively everything is known about it [2] and hence our approximation can be quantitatively tested). We are aware that the Ginzburg–Landau limit ($T \to T_C$) is not particularly realistic for this system, owing to an extremely high transition temperature $\sim 10^4$ K. However, this is included for completeness. In other physical systems it is a region of considerable physical interest.

In section 2, we integrate out the fermions and express the free energy in terms of a proper-time integral representation involving only the order parameter. In section 3, we consider the system with a single topological soliton present and describe in detail an approximation for the free energy. In section 4, we calculate the free energy associated with a soliton (for definiteness at zero temperature). Section 5 consists of a table of results and a discussion of various features of the approximation along with a comparison of our results with known exact results. Three appendices are included, which show the divergence cancellation of the free energy in the weak-coupling limit, the connection of the present work with Ginzburg–Landau theory and a representation of the heat kernel.

2. Expressing the free energy in the proper-time representation

The free energy F of polyacetylene, relative to the free energy of a uniformly dimerized system F_0 (with the gap $\Delta = \Delta_0$), is found, in the static dimerization approximation, from the ratio of Grassmann functional integrals [2]

$$\exp[-\beta(F - F_0)] = \frac{\int [\mathrm{d}\bar{\psi}]\,[\mathrm{d}\psi]\,\mathrm{e}^{-S}}{\int [\mathrm{d}\bar{\psi}]\,[\mathrm{d}\psi]\,\mathrm{e}^{-S_0}} \tag{2.1}$$

with

$$S = \int_0^\beta L\,\mathrm{d}\tau + \frac{\omega_Q^2}{2g^2}\beta \int \mathrm{d}x\,\Delta(x)^2 \tag{2.2a}$$

$$L = \int \mathrm{d}x\,\bar{\psi}(\partial_\tau + H)\psi \tag{2.2b}$$

$$H = -\mathrm{i}v_F\sigma_3\partial_x + \Delta(x)\sigma_1 \tag{2.2c}$$

where β is the reciprocal of the temperature T and τ is a Euclidean time variable. A quantity with subscript 0 is obtained from the above by replacing $\Delta(x)$ by Δ_0. The dimerization field Δ is static in the present work; it depends only on x and not on τ. In (2.2*a*) ω_Q and g are effective spring and coupling constants for the dimerization. The Fermi velocity is denoted by v_F and σ_k ($k = 1, 2, 3$) are the Pauli matrices, which describe the physics in the problem associated with electrons moving at $\pm v_F$ (they do not describe the spin, which plays an almost passive role in what follows and merely results in a factor of 2 appearing).

The functional integrals can be carried out and lead to

$$\exp[-\beta(F - F_0)] = \left(\frac{\mathrm{Det}[\partial_\tau + H]}{\mathrm{Det}[\partial_\tau + H_0]}\right)^2 \exp\left[\frac{-\beta\omega_Q^2}{2g^2}\int \mathrm{d}x\,(\Delta^2 - \Delta_0^2\right] \tag{2.3}$$

where the power of 2 follows from the spin multiplicity. The determinants are evaluated on eigenfunctions that are antiperiodic in τ over $[0, \beta]$. As is discussed in [2], it is possible to replace $\mathrm{Det}[\partial_\tau + H]$ by $(\mathrm{Det}[-\partial_\tau^2 + H^2])^{1/2}$; thus we can write

$$F - F_0 = -\frac{1}{\beta}\ln\left(\frac{\mathrm{Det}[-\partial_\tau^2 + H^2]}{\mathrm{Det}[-\partial_\tau^2 + H_0^2]}\right) + \frac{\omega_Q^2}{2g^2}\int \mathrm{d}x\,(\Delta^2 - \Delta_0^2). \tag{2.4}$$

Using the identity between determinants and traces

$$\ln \mathrm{Det}(\ldots) = \mathrm{Tr}\ln(\ldots) \tag{2.5}$$

we can write

$$F - F_0 = -\frac{1}{\beta}\mathrm{Tr}\ln\left(\frac{-\partial_\tau^2 + H^2}{-\partial_\tau^2 + H_0^2}\right) + \frac{\omega_Q^2}{2g^2}\int \mathrm{d}x\,(\Delta^2 - \Delta_0^2). \tag{2.6}$$

If we use the following integral representation for $\ln(x/y)$, with both x and y positive numbers,

$$\ln(x/y) = -\int_0^\infty \frac{\mathrm{d}s}{s}(\mathrm{e}^{-sx} - \mathrm{e}^{-sy}) \tag{2.7}$$

(which may be explicitly verified by differentiating with respect to x or y) we can write

$$F - F_0 = \frac{1}{\beta}\mathrm{Tr}\int_0^\infty \frac{\mathrm{d}s}{s}\{\exp[-s(-\partial_\tau^2 + H^2)] - \exp[-s(-\partial_\tau^2 + H_0^2)]\} + \frac{\omega_Q^2}{2g^2}\int \mathrm{d}x\,(\Delta^2 - \Delta_0^2). \tag{2.8}$$

Note that the trace Tr that appears in this equation is to be understood in the functional sense, i.e.

$$\mathrm{Tr}(\ldots) = \mathrm{tr}\int \mathrm{d}x \int_0^\beta \langle x, \tau|(\ldots)|x, \tau\rangle$$

where tr is the trace over the internal matrix space (which has different interpretations in different systems, c.f. the comments in section 1). Thus

$$F - F_0 = \frac{1}{\beta}\mathrm{tr}\sum_n \int_0^\infty \frac{\mathrm{d}s}{s}\mathrm{e}^{-s\omega_n^2}\int \mathrm{d}x\,\langle x|(e^{-sH^2} - e^{-sH_0^2})|x\rangle + \frac{\omega_Q^2}{2g^2}\int \mathrm{d}x\,(\Delta^2 - \Delta_0^2) \tag{2.9}$$

where $\omega_n = (2n + 1)\pi T$ are the Matsubara frequencies that enforce antiperiodicity in τ.

We shall refer to s as the proper time and to equation (2.9) as the proper-time representation of the free energy. We shall also refer to the quantity

$$K(s) = \mathrm{tr} \int \mathrm{d}x \, \langle x|(\mathrm{e}^{-sH^2} - \mathrm{e}^{-sH_0^2})|x\rangle \tag{2.10}$$

appearing in equation (2.9) as the integrated heat kernel.

The integral representation of $\ln(A/B)$ was first (to our knowledge) used in physics by Schwinger in a remarkable paper where he was able to carry out perturbative calculations in quantum electrodynamics (QED) in a gauge-invariant way [3]. Although it may not be manifest in what follows, our results also possess the property of gauge invariance and thus the method can be generalized to systems involving electromagnetic fields [4].

3. The approximation for the free energy in the one-soliton sector

From the previous section we see that the free energy can be expressed solely in terms of the order parameter Δ, albeit as a complicated functional form. In this section we are going to consider the case where F refers to the system that possesses a single topological soliton and F_0 refers to the uniform system. We discuss an approximation scheme for the free energy that generalized the results of D'yakanov *et al* [5] that were used in the very different context of quantum chromodynamics. We obtain the results necessary to evaluate the free energy of a soliton of given profile but with an arbitrary scale of spatial variation at an arbitrary temperature.

The proper-time representation for $F - F_0$ involves, *inter alia*, an s integration of the heat kernel $K(s)$ (equation (2.10)). We introduce a partition point δ, which separates two different regions of the parameter s, and we introduce different approximation schemes for each region. (The parameter s roughly corresponds to an inverse temperature and it is sometimes useful to call $s < \delta$ and $s > \delta$ high- and low-energy regions respectively).

The approximation we make aims to capture the essentially different behaviour of the heat kernel in the two regions. Thus we write

$$K(s) = \begin{cases} K_{\mathrm{H}}(s) & s < \delta \\ K_{\mathrm{L}}(s) & s > \delta. \end{cases} \tag{3.1}$$

This approximation is as follows:

(i) In the small s region, $s < \delta$, the heat kernel is expanded in ascending (fractional) powers of s, which is called the Minakshisundaran–Seeley (MS) coefficient expansion [6]. The approximation to $K_{\mathrm{H}}(s)$ consists of including only a finite number of terms in the expansion. The complexity of these terms increases rapidly with order and this provides a practical limit to the number of MS terms computed.

(ii) In the large s region, $s > \delta$, the approximation for the heat kernel consists of including only the low-lying modes of the operator H^2 in the summation over the eigenvalues. In the present work, we include only the bound states.

(iii) The approximation is fully specified by providing a prescription for the determination of the partition point δ that separates the low and high s behaviours. We note that the exact heat kernel is a continuous function of the proper time s. In general, the approximations embodied in (i) and (ii) above will not lead to a continuous function of s at $s = \delta$. The prescription we adopt is to select δ such that the mismatch of the two

approximations at $s = \delta$ is minimized. That is $[K_H(s) - K_L(s)]^2$ takes on its minimum value at $s = \delta$. (In many cases that we have considered the approximations for K_H and K_L can actually cross and hence a δ can be found such that we obtain a continuous approximation to $K(s)$.)

We note that (*a*) when no such minimum can be found it is necessary to include a large number of the MS expansion and (*b*) when there exists more than one δ that minimizes the mismatch, best results follow from taking the smaller root due to the improved convergence of the MS series.

Proceeding with the calculation, we return to equation (2.9) and evaluate, in the approximation described above, the excess free energy $F - F_0$ associated with the single soliton. We take the soliton profile to be given by

$$\Delta(x) = \Delta_0 \tanh(x\Delta_0/v_F\lambda) \tag{3.2}$$

where Δ_0 is the uniform dimerization amplitude and λ is a parameter that characterizes the size of the soliton (it is with hindsight that we parametrize the scale of spatial variation in this way; the free energy takes on a particularly simple form in the terms of λ).

From equation (2.2*c*) we have

$$H^2 = -v_F^2\partial_x^2 + \Delta^2(x) + \sigma_2 v_F \partial_x \Delta(x) \tag{3.3a}$$

$$H_0^2 = -v_F^2\partial_x^2 + \Delta_0^2. \tag{3.3b}$$

Introducing the partition point δ, we write the approximation soliton free energy, $(F - F_0)_{approx}$, as

$$(F - F_0)_{approx} = T\sum_n \left(\int_\eta^\delta \frac{ds}{s} e^{-\omega_n^2 s} K_H(s) + \int_\delta^\infty \frac{ds}{s} e^{-\omega_n^2 s} K_L(s) \right) + \frac{\omega_Q^2}{2g^2} \int dx\, (\Delta^2 - \Delta_0^2). \tag{3.4a}$$

Note that the effects of the finite electron bandwidth W have been incorporated into this equation by putting a lower limit of η onto the leading integral of equation (3.4). While the most obvious way to implement a cut-off is to restrict momentum integrals implicit in the above equation, appendix B of [2] discusses a number of equivalent ways the cut-off can be introduced. This stems from the fact that the physics of the soliton is intrinsically that of low energies and that the soliton free energy is insensitive to the precise method by which the high energies are cut off, and cutting off very small values of s is equivalent to cutting off high energies. From appendix B of [2] we have

$$\eta = (2e^{-\gamma/2}/W)^2 \tag{3.4b}$$

where W is the electron bandwidth and γ is Euler's constant.

In appendix 1, we show that what appear to be divergences associated with the weak-coupling limit $\Delta_0/W \to 0$ cancel between the elastic and high-energy contributions to the free energy. We shall, in what follows, neglect corrections to the free energy that are $O((\Delta_0/W)^n)$ with $n \geq 1$. That is, we work to zeroth order in the weak-coupling expansion. For realistic values of Δ_0/W the errors caused by this truncation are beyond the accuracy of our approximation to the free energy and therefore are insignificant in the present work.

3.1. High-energy contribution

Let us now determine the high-energy (small s) contribution to the heat kernel $K(s)$ appearing in equation (2.10). We first obtain an exact representation for $K(s)$ by taking

the configuration part of the trace in coordinate space; since H^2 and H_0^2 depend only of σ_2 it is convenient to take the spin part of the trace in a basis in which this matrix is diagonal. We obtain

$$K(s) = \sum_{\nu=+,-} \int dx \, \langle x|\exp(-\Omega_0 s) - \exp(-\Omega_0 s)|x\rangle \tag{3.5a}$$

where we have gone to an operator notation ($\hat{}$ denote operators)

$$\Omega_\nu = v_F^2 \hat{p}^2 + U_\nu \tag{3.5b}$$

$$U_\nu = (\Delta_0/\lambda)^2[\lambda^2 - \lambda(\lambda + \nu)\,\mathrm{sech}^2(\Delta_0 \hat{x}/\lambda v_F)] \qquad \nu = +1, -1 \tag{3.5c}$$

$$\Omega_0 = v_F^2 \hat{p}^2 + \Delta_0^2. \tag{3.5d}$$

In appendix 3 we show that equation (3.5*a*) may be written as

$$K(s) = \sum_\nu \int \frac{dp\,dx}{2\pi} \exp(-p^2 v_F^2 s)\,\{\exp[(v_F^2 \partial_x^2 + 2iv_F^2 p\partial_x - U_\nu)s] - \exp(-\Delta_0^2 s)\} \tag{3.6}$$

A small s expansion to $K(s)$ is obtained by expanding the curly bracket in equation (3.6), performing the integral over the momentum and then collecting together terms of the same power in s. The high-energy approximation to $K(s)$ is made by truncating this series at a finite order. We find

$$K_H(s) = \frac{1}{2\sqrt{\pi}} \int dx \sum_{k=0} [a_k(x) - a_k^{(0)}(x)] s^{(k-\frac{1}{2})} \tag{3.7}$$

where the a_k and $a_k^{(0)}$ are the MS coefficients corresponding to the soliton and soliton-free sectors respectively, and are given by

$$\begin{aligned}
a_0(x) - a_0^{(0)}(x) &= 0 \\
a_1(x) - a_1^{(0)}(x) &= \frac{1}{v_F} \sum_\nu (U_\nu + \Delta_0^2) \\
a_2(x) - a_2^{(0)}(x) &= \frac{1}{v_F} \sum_\nu \tfrac{1}{2}(U_\nu^2 - \Delta_0^4) \\
a_3(x) - a_3^{(0)}(x) &= \frac{1}{v_F} \sum_\nu \tfrac{1}{6}(U_\nu^3 + \Delta_0^6 + \tfrac{1}{2} v_F^2 U_\nu \partial^2 U_\nu) \\
a_4(x) - a_4^{(0)}(x) &= \frac{1}{v_F} \sum_\nu \tfrac{1}{120}[5(U_\nu^4 - \Delta_0^8) - 5v_F^2 U_\nu^2 \partial_x^2 U_\nu + v_F^4 U_\nu \partial_x^4 U_\nu].
\end{aligned} \tag{3.8}$$

On substituting for the U_ν and integrating over x we find that a simple form for $K_H(s)$ is obtained by expressing the results in terms of the dimensionless variable t defined by

$$s = (\lambda/\Delta_0)^2 t. \tag{3.9}$$

We obtain a series in powers of t with dimensionless coefficients A_k, which follow form equation (3.8):

$$K_H(s) \equiv K_H((\lambda/\Delta_0)^2 t) = \frac{1}{2\sqrt{\pi}} \sum_{k=1} A_k(\lambda) t^{(k-\frac{1}{2})} \tag{3.10}$$

with

$$\begin{aligned}
A_1 &= 4\lambda^2 \\
A_2 &= \tfrac{8}{3}\lambda^2(1 - 2\lambda^2) \\
A_3 &= \tfrac{2}{15}\lambda^2(23\lambda^4 - 10\lambda^2 - 4) \\
A_4 &= \tfrac{2}{315}\lambda^2(-\tfrac{44}{21}\lambda^6 + \lambda^4 + \tfrac{8}{21}).
\end{aligned} \tag{3.11}$$

3.2. Low-energy contribution

Let us now consider the low-energy part of the heat kernel, $K_L(s)$. Owing to the presence of the soliton, the operators $\Omega_\pm$ appearing in H^2 have discrete bound states [1]. The bound-state spectra of $\Omega_\pm$ differ in that Ω_+ has an exact zero mode whereas Ω_- does not. The non-zero bound states of $\Omega_\pm$ are $E_n = (\Delta_0/\lambda)^2\,(2\lambda n - n^2)$, where n is integral and $[\lambda] \geqslant n \geqslant 1$. The continua of $\Omega_\pm$ and Ω_0 correspond to energies $\geqslant \Delta_0^2$.

In our approximation we will assume that only the bound states contribute to $K_L(s)$, assuming that the difference in the continuum parts of the spectrum between the soliton and soliton-free sectors is taken into account in $K_H(s)$. Thus

$$K_L(s) = 1 + 2\sum_{n=1}^{[\lambda]} e^{-E_n s}. \tag{3.12}$$

This quantity, like $K_H(s)$, takes on a simple form when expressed in terms of t given in equation (3.9):

$$K_L(s) \equiv K_L((\lambda/\Delta_0)^2 t) = 1 + 2\sum_{n=1}^{[\lambda]} \exp[-(2\lambda n - n^2)t]. \tag{3.13}$$

3.3. Determination of the partition point

As noted above, the partition point is chosen in such a way that $[K_H(s) - K_L(s)]^2$ is minimized at $s = \delta$, i.e.

$$(d/ds)[K_H(s) - K_L(s)]^2|_{s=\delta} = 0. \tag{3.14}$$

If we go to a dimensionless variable ε related to δ in the same way that t is related to s:

$$\delta = (\lambda/\Delta_0)^2\varepsilon \tag{3.15}$$

then there is the very significant advantage that ε is independent of Δ_0. (This is most easily seen by re-expressing equation (3.14) in terms of t and ε.) Since the equation that determines ε, equation (3.14), in independent of ω_n and Δ_0, it follows that ε is independent of temperature. Thus a numerical solution of equation (3.14) is sufficient to determine the free energy for all temperatures. In table 1 we give the dimensionless partition point ε for a range of values of λ. The approximation to the free energy is thus

$$(F - F_0)_{\text{approx}} = T\sum_n \left(\int_{\eta(\Delta_0/\lambda)^2}^{\varepsilon} \frac{dt}{t} \exp[-(\lambda\omega_n/\Delta_0)^2 t] K_H((\lambda\omega_n/\Delta_0)^2 t) \right.$$
$$\left. + \int_{\varepsilon}^{\infty} \frac{dt}{t} \exp[-(\lambda\omega_n/\Delta_0)^2 t] K_L((\lambda\omega_n/\Delta_0)^2 t) \right) - \frac{v_F^2\omega_Q^2}{g^2}\Delta_0\lambda. \tag{3.16}$$

4. The soliton creation energy

The results of the previous section can be used to find the free energy associated with a soliton for arbitrary values of T and λ. In order to decrease the number of parameters under consideration, we specialize to the case $T = 0$. This choice has been made only for definiteness and ease of comparison with existing results. The only simplification that occurs in this limit is that we have to contend with integrals instead of sums over the Matsubara frequencies. The zero-temperature limit of the soliton free energy is the

Table 1. The approximate soliton free energy is given for three and four MS coefficients and for various values of the 'size' parameter λ. These are compared with the exact free energy, which can be calculated analytically at integral values of λ. It is evident that the accuracy of the approximation increases with the number of MS coefficients included.

		Three MS terms		Four MS terms		
λ	Number of bound states	ε	$(E-E_0)/\Delta_0$	ε	$(E-E_0)/\Delta_0$	Exact $(E-E_0)/\Delta_0$
0.2	1	4.677	1.292	8.375	1.156	0.772
0.4	1	3.476	0.813	5.084	0.802	0.694
0.6	1	2.594	0.694	3.565	0.697	0.657
0.8	1	2.427	0.646	2.787	0.655	0.641
1.0	1	1.493	0.650	1.596	0.640	0.637
1.0	2	2.149	0.671	2.217	0.644	0.637
2.0	2	0.357	0.757	0.372	0.715	0.696
6.0	6	0.041	1.471	0.043	1.310	1.238

soliton creation energy and will be denoted by $(E-E_0)_{\text{approx}}$. The quantity is the zero-temperature limit of equation (3.16).

The steps leading to the soliton creation energy are as follows. We perform the integrals over ω_n and t in equation (3.16). Using the $T=0$ uniform dimerization amplitude [1, 2]

$$\Delta_0 = W\exp(-\pi v_F\omega_Q/2g^2) \tag{4.1}$$

the elastic term is expressed in terms of Δ_0/W. Finally working to zeroth order in the weak-coupling parameter Δ_0/W we obtain the soliton creation energy in terms of the 'size' parameter λ and the dimensionless partition point ε:

$$\begin{aligned}\frac{(E-E_0)_{\text{approx}}}{\Delta_0} &= \frac{\lambda}{\pi}[\log(\lambda^2\varepsilon)+\gamma] + \lambda\left(\frac{1-2\lambda^2}{3\pi}\right)\varepsilon + \frac{\lambda}{180\pi}(23\lambda^4-10\lambda^2-4)\varepsilon^2 \\ &\quad + \frac{\lambda}{90\pi}(-\tfrac{44}{21}\lambda^6+\lambda^4+\tfrac{8}{21})\varepsilon^3 + \frac{1}{(\pi\lambda^2\varepsilon)^{1/2}} \\ &\quad + \frac{1}{(\pi\lambda^2)^{1/2}}\sum_{n=1}^{[\lambda]}\int_\varepsilon^\infty \frac{\mathrm{d}t}{t^{3/2}}\,\mathrm{e}^{-(2\lambda n-n^2)t}.\end{aligned} \tag{4.2}$$

5. Results and discussion

In this section we present a detailed analysis of results for our approximation for the free energy. We calculate the soliton creation energy (referred to in this section as the free energy) for various values of λ with three and four MS coefficients. These are used to find the approximate minimum of the free energy. The approximation is also investigated for large values of λ where there are a large number of bound states. These results are compared with the exact calculation of [2].

In table 1 we give the approximate soliton free energy (calculated with three and four MS coefficients), the partition point $\varepsilon(\lambda)$ and the exact soliton creation energy, all evaluated for a range of values of λ. The discontinuity in $(E-E_0)_{\text{approx}}$ at integer values of λ arises since new bound states are generated as λ passes through an integer. A

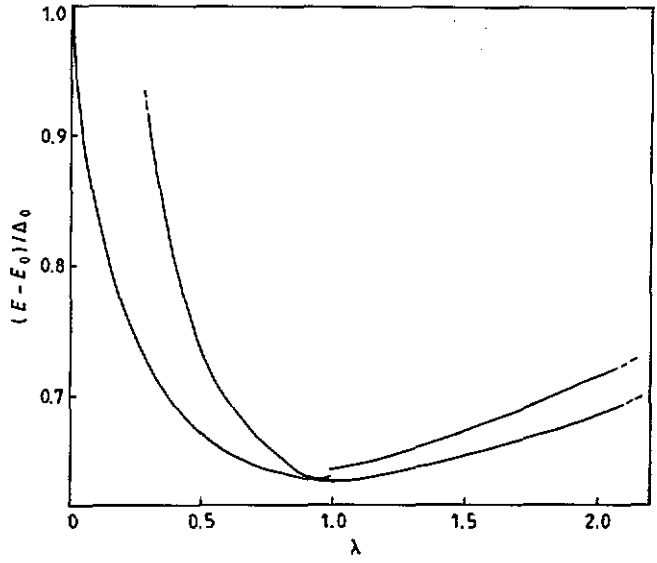

Figure 1. The exact soliton creation energy (lower curve) and the approximate soliton creation energy (upper curve) are plotted for a range of values of the 'size' parameter λ. The approximation for the creation energy was obtained when four MS coefficients were included in the calculation. The discontinuity appearing in the curve for the approximation at $\lambda = 1$ results from a new bound state being trapped on the soliton. A smoothing out of the density of bound states would avoid this feature [8].

continuous approximation can be obtained by smoothing out the delta functions in the density of bound states. We have not carried out this smoothing in the present work since it requires detailed consideration of the low-lying scattering states; this will be discussed elsewhere [8].

While we have treated the parameter λ as arbitrary, its physical value corresponds to the minimum of the free energy. Exact calculations [2] show that this value is unity. It is interesting to see how close our approximation can come to this value. The minimum of the approximate free energy is shallow so that the error in the value of λ at the minimum can be much larger than the error in the approximate free energy. We find that for three MS coefficients the partition point discontinuously exchanges minima of $(K_H - K_L)^2$ as λ passes through 0.8543, and as a consequence the approximate free energy has a small discontinuity at this value of λ. In what appears to be a coincidence, this value of λ also yields the free energy minimum with $(E - E_0)_{approx} = 0.6288\Delta_0$ when λ approaches 0.8543 from below. The discontinuity in the free energy (<1%) is smaller than the error on the minimum value of the free energy (1.2%). This behaviour is not quite satisfactory; however, we find that by including four MS coefficients the free energy is continuous for all non-integral values of λ. In particular with four MS coefficients the free energy has a smooth minimum at $\lambda = 0.9050$ and achieves a value of $(E - E_0)_{approx} = 0.6385\Delta_0$, corresponding to errors on λ and the free energy of 9.5% and 0.3% respectively. In figure 1 the exact soliton creation energy along with our approximation (calculated for four MS coefficients) are plotted for a range of values of λ.

It is instructive to make a comparison between the accuracy of the approximation and the convergence of the proper-time expansion used in the free energy. For this purpose let us write $(E - E_0)_{high} = \Sigma(E - E_0)^{(n)}_{high}$, where the subscript 'high' refers to the high-energy (small s) contribution to the free energy and the superscript '(n)' refers

Table 2. The relative contributions of the successive terms to the high-energy part of the approximation to the free energy are given. The accuracy of the approximation increases with the degree of convergence of the high-energy expansion.

Three MS terms.

λ	Number of bound states	$(E-E_0)^{(n)}/\Delta_0$ $n=1$	$n=2$	$n=3$
0.2	1	−0.070	0.091	−0.034
0.4	1	−0.001	0.100	−0.043
0.6	1	0.097	0.046	−0.033
0.8	1	0.259	−0.058	−0.008
1.0	1	0.311	−0.158	0.035
1.0	2	0.427	−0.228	0.074
2.0	2	0.594	−0.530	0.146
6.0	6	1.865	−1.871	0.535

Four MS terms.

λ	Number of bound states	$(E-E_0)^{(n)}/\Delta_0$ $n=1$	$n=2$	$n=3$	$n=4$
0.2	1	−0.033	0.164	−0.108	0.159
0.4	1	0.047	0.147	−0.092	0.074
0.6	1	0.158	0.064	−0.062	0.040
0.8	1	0.294	−0.066	−0.011	0.015
1.0	1	0.333	−0.169	0.041	−0.010
1.0	2	0.437	−0.235	0.078	−0.026
2.0	2	0.620	−0.553	0.159	−0.043
6.0	6	1.933	−1.939	0.575	−0.162

to the contribution to the nth MS coefficient. In table 2 we give values for $(E-E_0)^{(n)}_{\text{high}}$ for various values of λ, again with three and four MS coefficients. Inspection of table 2 shows that the accuracy of the approximation to the free energy is measured by the degree of convergence of the MS expansion. Best results are obtained when the ratio of successive terms in $(E-E_0)_{\text{high}}$ is small, and this gives a straightforward check on the minimum number of MS coefficients necessary for a reasonable result. (The MS expansion is, for general values of λ, likely to be asymptotic and thus will diverge if summed to all orders. This situation is very similar to perturbative expansions in QED.)

To summarize, the methods presented in this paper allow the calculation of the free energy for a class of fermionic systems involving extended order parameter structures (solitons). The method works to a good accuracy over the entire temperature range 0 to T_C. Thus even at low temperatures where highly non-local quantum effects are present and no simple free energy functional (e.g. of a Ginzburg–Landau type) exists, the method is able to produce results of good accuracy. The method presented is quite general in that the MS series is straightforward to obtain irrespective of dimensionality and the complexity of the Hamiltonian. Furthermore, even in cases where the bound states cannot be calculated exactly, there are many techniques for their approximate calculation.

Having tested the method in an exactly solvable model problem we plan, elsewhere, to apply it to more complex systems.

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Appendix 1. Divergence cancellation

In this appendix, we show that divergences associated with the extreme weak-coupling limit, $\Delta_0/W \to 0$, cancel between the electronic and elastic pieces of the free energy. We find it convenient to incorporate the bandwidth cut-off, ω, in the frequency sum instead of the proper time integral (see appendix B of [2]). Thus the frequency sums run up to N where N is given by $W = 2\pi T(2N \pm 1)$ and the lower limit of the proper time integral is set to zero. From equations (3.10) and (3.16), it is straightforward to see that if $\mathcal{O}(((\Delta_0/W)^n)$, $n \geqslant 1$, contributions are neglected then the only dependence on Δ_0/W in the electronic part of the free energy comes from the first term of the MS expansion. Also the elastic part of the free energy retains a dependence on Δ_0/W, through the uniform dimerization equation

$$\frac{v_F \omega_Q^2}{g^2} = 4T \sum_{n=0}^{N} \frac{1}{(\omega_n^2 + \Delta_0^2)^{1/2}}. \tag{A1.1}$$

This equation is a trivial generalization of the zero-temperature result obtained in [2]. Combining these two contributions, we have

$$\frac{1}{\sqrt{\pi}} \int_0 \frac{\varepsilon \, d\bar{s}}{\bar{s}} T \sum_{n=0}^{N} \exp[-(\lambda \omega_n/\Delta_0)^2 \bar{s}] A_1 \bar{s}^{1/2} - \frac{v_F \omega_Q^2}{g^2} \lambda \Delta_0. \tag{A1.2}$$

Integrating over $\bar{s}$ and substituting for A_1, equation (3.11), we find that equation (A1.2) becomes

$$4T\lambda \sum_{n=0}^{N} \left[\frac{\Delta_0}{\omega_n} \operatorname{erf}\left(\lambda \frac{\omega_n}{\Delta_0} \sqrt{(\varepsilon)} \right) - \frac{1}{[1 + (\omega_n/\Delta_0)^2]^{1/2}} \right]. \tag{A1.3}$$

As N tends to infinity, the divergences in the two terms in equation (A.3) cancel. A consequence of this is that in the weak coupling limit, $\Delta_0/W \ll 1$, $(F - F_0)/\Delta_0$ may be accurately approximated by working to zeroth order in Δ_0/W.

Appendix 2. Ginzburg–Landau analysis

In this appendix, we present the high-temperature ($T \to T_C$) Ginzburg–Landau limit for the free energy. The closest connection to the derivation given in this appendix is with the work of Schakel [7].

The Ginzburg–Landau form for the free energy arises, in the language of proper-time integrals, only from small s. This has the consequence that any low-energy modes

(e.g. bound states) make a negligible contribution to the free energy. Thus only the MS coefficients in the high-energy piece $K_H(s)$ and the elastic term significantly contribute to the free energy, resulting in a free energy that is a simple functional of the order parameter. (This is in sharp contrast to the case of low temperatures where the low-lying spectrum and hence the form of the free energy depend in a highly non-trivial way on the profile of the order parameter.)

The fact that only the small s region contributes to the free energy arises from the following rather general observation: the partition point δ appearing in equation (3.4*a*) has the dimensions of (energy)$^{-2}$. From the definition of δ it follows that it does not depend explicitly on temperature. There is then effectively only one energy scale available for it to depend upon, namely Δ_0. Consequently $\delta\Delta_0^2$ is $\mathcal{O}(1)$ for all temperatures $T < T_C$. Thus, $\delta \sim \Delta_0^{-2}$ becomes very large for $T \lesssim T_C$ and the factor $\exp(-\omega_n^2 s)$ in equation (3.4*a*) exponentially suppresses $s > \delta$ contributions to the free energy. It follows that it is a good approximation to replace δ by infinity in equation (3.4*a*). Thus we have for $T \lesssim T_C$ (again we put the cut-off in the frequency sum, see appendix 1)

$$(F - F_0)_{\text{approx}} = T \sum_{n=0}^{N} \int_0^\infty \frac{ds}{s} e^{-\omega_n^2 s} K_H(s) + \frac{\omega_0^2}{2g^2} \int dx\, [\Delta^2(x) - \Delta_0^2]. \tag{A2.1}$$

Using the results of equations (3.9) and (3.10) we can write

$$2T \sum_{n=0}^{N} \frac{ds}{s} e^{-\omega_n^2 s} K_H(s) = T \sum_{n=0}^{N} \frac{1}{v_F} \left(\frac{1}{\omega_n} \int dx\, 2(\Delta^2 - \Delta_0^2) + \frac{1}{2\omega_n^3} \int dx\, [\Delta^4 + (v_F \partial_x \Delta)^2 - \Delta_0^4] \right). \tag{A2.2}$$

The first sum above depends logarithmically on N and hence the cut-off W. It is adequate (since $N \gg 1$) to use

$$\sum_{n=0}^{N} \frac{1}{2n+1} = \tfrac{1}{2} \ln\left(\frac{W}{\pi T}\right) + \gamma + \mathcal{O}(T/W) \tag{A2.3}$$

where we have recalled that $(2N+1)\pi T = W/2$ and γ is Euler's constant.

The second sum in equation (A2.2) is highly convergent and we make the excellent approximation of taking its upper limit to be infinity. Hence

$$2T \sum_{n=0}^{N} \int \frac{ds}{s} e^{-\omega_n^2 s} K_H(s) = -\frac{1}{\pi v_F} \ln\left(\frac{W}{\pi T} e^{\gamma}\right) \int dx\, (\Delta^2 - \Delta_0^2) + \frac{7\zeta(3)}{16\pi^3 v_F T^2} \times \int dx\, [\Delta^4 + v_F^2 (\partial_x \Delta)^2 - \Delta_0^4] + \mathcal{O}(T^{-4}) \tag{A2.4}$$

where $\zeta(z)$ is Riemann's ζ-function. Provided we are close enough to T_C and spatial variations of $\Delta(x)$ are smooth we can neglect the $\mathcal{O}(T^{-4})$ corrections. Substituting for $(a_1 - a_1^{(0)})$ and $(a_2 - a_2^{(0)})$ from equation (3.8), and setting $T = T_C$ in the coefficient of $(a_2 - a_2^{(0)})$, we find

$$(F - F_0)_{\text{approx}} = -\frac{1}{\pi v_F} \ln\left(\frac{T_C}{T}\right) \int dx\, (\Delta^2 - \Delta_0^2) + \frac{7\zeta(3)}{16\pi^3 v_F T_C^2} \times \int dx\, [\Delta^4 - v_F^2 (\partial_x \Delta)^2 - \Delta_0^4] \tag{A2.5}$$

where we have defined the critical temperature T_C as the temperature at which the coefficient of Δ^2 vanishes. It is determined from

$$\frac{2}{\pi}\ln\left(\frac{W}{\pi T_C}e^{\gamma}\right)=\frac{\omega_Q^2 v_F}{g^2}. \tag{A2.6}$$

In this way we obtain the Ginzburg–Landau free energy functional with the uniform bulk free energy subtracted. If the unsubtracted free energy is required, then Δ_0 may be set to zero in equation (A2.5).

Let us note several points:

(i) The Ginzburg–Landau free energy is a simple functional (i.e. an integral of a local free energy density) of the order parameter. This is in sharp contrast to the case of low temperatures; the low-lying spectrum depends in a highly non-trivial way on the profile of the order parameter and in general we would exect an extremely complicated free energy functional.

(ii) The ratio of successive terms in the Ginzburg–Landau free energy is $\mathcal{O}((\Delta/T)^2)$. This makes it clear that it cannot be straightforwardly extended to low temperatures and detailed considerations such as those given in the main body of this work are necessary.

Appendix 3. Representation of the heat kernel

In this appendix we derive a representation for the heat kernel that has a natural expansion in powers of the proper-time variable s. Let us consider the quantity

$$A(x,x';s)=\langle x|\exp[-s(v_F^2\hat{p}^2+U_v)]|x'\rangle. \tag{A3.1}$$

Thus

$$-\partial_s A(x,x';s)=(-v_F^2\partial_x^2+U_v)A(x,x';s). \tag{A3.2}$$

Integrating this equation gives

$$A(x,x';s)=\exp[-s(-v_F^2\partial_x^2+U_v)]A(x,x';0). \tag{A3.3}$$

Noting that

$$A(x,x';0)=\delta(x-x')=\int\frac{dp}{2\pi}e^{ip(x-x')} \tag{A3.4}$$

and using the identity

$$\partial_x e^{ip(x-x')}\equiv e^{ip(x-x')}(\partial_x+ip) \tag{A3.5}$$

we can write equation (A3.3) as

$$A(x,x';s)=\int\frac{dp}{2\pi}e^{ip(x-x')}\exp\{-s[-v_F^2(\partial_x+ip)^2+U_v]\}. \tag{A3.6}$$

Thus

$$\int dx\,\langle x|\exp[-s(v_F^2\hat{p}^2+U_v)]|x\rangle=\int\frac{dp\,dx}{2\pi}\exp(-p^2v_F^2s)\exp[(v_F^2\partial_x^2+2iv_F^2p\partial_x-U_v)s]. \tag{A3.7}$$

Finally we note that if U_v in this equation is replaced by Δ_0^2, which is independent of x,

then the derivatives in the exponent have nothing to act upon and may be omitted. It then follows that

$$\int \mathrm{d}x \, \langle x| \exp[-s(v_F^2\hat{p}^2 + U_\nu)] - \exp[-s(v_F^2\hat{p}^2 + \Delta_0^2)] \, |x\rangle$$

$$= \int \frac{\mathrm{d}p \, \mathrm{d}x}{2\pi} \exp(-p^2 v_F^2 s) \{\exp[(v_F^2\partial_x^2 + 2iv_F^2 p\partial_x - U_\nu)s] - \exp(-\Delta_0^2 s)\} \tag{A3.8}$$

which is essentially equation (3.6).

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