J. Phys. A: Math. Gen. 26 (1993) 765–768. Printed in the UK

ADDENDUM

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

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Received 12 June 1992

Abstract. In the paper of the same title, the behaviour of the free energy was investigated for an exactly soluble condensed matter system that contained a topological soliton. When λ, the size of the soliton in units of the coherence length, was small compared with unity, the free energy was shown to behave as a non-analytic function of λ. In the present work we show that a simple approximation to the exact free energy exists which is able to reproduce the leading small λ results and, more generally, approximate the exact free energy, with reasonable accuracy, over a wide range of λ. Thus at zero temperature, for example, the errors the approximate free energy makes on the value of λ and the free energy at its minimum are 18% and 8.3% respectively.

1. Introduction

This addendum is a sequel to the earlier paper of the same title [1]. We assume that [1] has been read and the same notation will be used in the present work without additional explanations. We shall present additional results on the free energy associated with topological solitons in the linear molecule polyacetylene. In this system a kink or topological soliton (≡domain wall) in the dimerization field is coupled to a band of electrons in the molecule.

The free energy associated with a topological soliton (such as a domain wall) in a fermionic system arises from at least two different origins. (1) The fermions move in the field of the soliton and the soliton modifies their motion compared with a uniform system. The fermions are scattered and bound by the soliton. This results in a change of the fermionic spectrum and results in one contribution to the soliton free energy. (2) Another contribution arises from a pure 'order parameter' term (in polyacetylene the order parameter is the dimerization); when the order parameter deviates from its bulk value an energy change is incurred. Additional terms may be present in the free energy; however, in a 'mean field' type of theory (where fermions couple bilinearly to an order parameter) the two terms mentioned above are always present. The investigation of the two terms noted above therefore has applications in a number of systems. This provides the motivation for studying a model system and gaining additional insight into the factors that play a key role in the make-up of topological solitons.

It is evident that the exact determination of the structure of a topological soliton requires the detailed knowledge of the effects of the soliton on the fermionic spectrum

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0305-4470/93/030765+04$07.50

and, in general, this is difficult to find. Here we illustrate that a simple approximation exists that is able to reproduce the exact free energy, to a reasonable approximation, over a wide range of the 'size parameter' of the soliton λ. This quantity measures the soliton size in units of the coherence length $\xi_0 = v_F/\Delta_0$. For comparison with existing results [2] we shall work at zero temperature. We note that at low temperatures the free energy is an intrinsically non-local functional of the order parameter. It may be considered surprising that many of the long-ranged quantum correlations present in the system (which result in the non-local character of the free energy) are capturable by a relatively simple approximation, as we shall show.

2. Contribution to the soliton creation energy from quadratic terms in the 'potential'

The approximation to the free energy we present here consists of keeping terms of quadratic order in the 'potential'

$$V \equiv H^2 - H_0^2 \tag{1}$$

along with a correction term.

To begin we use equation (4.11) of [1] for the difference between the free energy of a soliton bearing system and that of a uniform system:

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

We specialize this equation to zero temperature, when $(F - F_0)$ becomes the soliton creation energy, which in units of the uniform dimerization is written, $(E - E_0)/\Delta_0$. The contribution to $(E - E_0)/\Delta_0$ that is quadratic in the potential V arises from the term in the sum over n with $n = 2$. It is

$$(E - E_0)^{(2)}/\Delta_0 = \frac{1}{4\pi} \int_0^\infty \mathrm{d}\nu \int \mathrm{d}y_1\, \mathrm{d}y_2 \frac{\exp(-2\lambda\sqrt{1+\nu^2}|y_1 - y_2|)}{(1+\nu^2)}$$
$$\times \{\Phi'(y_1)\Phi'(y_2) + \lambda^2[1 - \Phi^2(y_1)][1 - \Phi^2(y_2)]\}. \tag{3}$$

It is convenient to express $(E - E_0)^{(2)}/\Delta_0$ in terms of the Fourier transforms of $\Phi'(y)$, $[1 - \Phi^2(y)]$:

$$\chi_1(k) = \int \Phi'(y)\, \mathrm{e}^{\mathrm{i}ky}\, \mathrm{d}y \qquad \chi_2(k) = \int [1 - \Phi^2(y)]\, \mathrm{e}^{\mathrm{i}ky}\, \mathrm{d}y \tag{4}$$

and in terms of these,

$$(E - E_0)^{(2)}/\Delta_0 = \frac{1}{4\pi^2\lambda} \int_0^\infty \mathrm{d}\nu \int_0^\infty \mathrm{d}k \frac{1}{\sqrt{1+\nu^2}} \frac{1}{1 + \nu^2 + (k/2\lambda)^2} \{|\chi_1(k)|^2 + \lambda^2|\chi_2(k)|^2\}. \tag{5}$$

On evaluating the frequency integral and replacing k by the variable

$$a = k/(2\lambda) \tag{6}$$

we obtain the following representation of $(E - E_0)^{(2)}/\Delta_0$:

$$(E - E_0)^{(2)}/\Delta_0 = \frac{1}{2\pi^2} \int_0^\infty \mathrm{d}a \frac{1}{a\sqrt{1+a^2}} \ln(a + \sqrt{1+a^2}) \{|\chi_1(2\lambda a)|^2 + \lambda^2|\chi_2(2\lambda a)|^2\}. \tag{7}$$

3. Comparison of $(E-E_0)^{(2)}/\Delta_0$ with the limiting behaviour of the exact soliton creation energy

In [1] the limiting behaviour of the soliton creation energy was determined in the limit $\lambda \to 0$. It was found that

$$(E-E_0)/\Delta_0 \approx 1+\alpha_1 \lambda \ln \lambda + \alpha_2 \lambda + \ldots \qquad \lambda \to 0 \tag{8}$$

where the coefficients α_1 and α_2 are functionals of the profile $\Phi(y)$. It follows from [1] that in the small λ limit the non-trivial $\lambda \ln \lambda$ and λ dependence comes solely from the term in the free energy that is quadratic in the potential V. Thus any approximation to the free energy that includes the term in V^2 is guaranteed to correctly incorporate all the non-constant small λ behaviour up to order $\lambda \ln \lambda$ and λ. By contrast the contribution of unity to $(E-E_0)/\Delta_0$ that appears in equation (8) arises from an infinite summation over all powers of the potential V [1]. From equation (7) we can determine the $\lambda \to 0$ limit of $(E-E_0)^{(2)}/\Delta_0$. In the limit $\lambda \to 0$ we replace $\{|\chi_1(2\lambda a)|^2+\lambda^2|\chi_2(2\lambda)a)|^2\}$ by $|\chi_1(0)|^2$ and furthermore since $\Phi(\pm\infty)=\pm 1$

$$|\chi_1(0)|^2 = \left(\int \mathrm{d}y\, \Phi'(y)\right)^2 \equiv 4. \tag{9}$$

The remaining integral is standard and results in

$$(E-E_0)^{(2)}/\Delta_0|_{\lambda=0} = \tfrac{1}{2}. \tag{10}$$

We thus see that the quantity $(E-E_0)^{\text{approx}}/\Delta_0$ defined by

$$(E-E_0)^{\text{approx}}/\Delta_0 = 0.5+(E-E_0)^{(2)}/\Delta_0 \tag{11}$$

behaves for small λ precisely as the exact free energy given in equation (8).

We can furthermore show that at large values of λ, $(E-E_0)^{\text{approx}}/\Delta_0$ has the qualitatively correct behaviour; it increases linearly with λ as does the exact result [3]. To see this we note that for $\lambda \to \infty$ the rapid falloff of the Fourier transforms χ_1, χ_2 in equation (10) forces the integration variable a to be $\leqslant \lambda^{-1}$. We can then expand $\ln(a+\sqrt{1+a^2})/a\sqrt{1+a^2}$ to leading order in a:

$$\ln(a+\sqrt{1+a^2})/a\sqrt{1+a^2} = 1+\mathrm{O}(a^2). \tag{12}$$

Reverting back to a real-space representation we find

$$(E-E_0)^{\text{approx}}/\Delta_0|_{\lambda \gg 1} = \left(\frac{1}{4\pi}\int_{-\infty}^{\infty} \mathrm{d}y[1-\Phi^2(y)]^2\right)\lambda + \mathrm{O}(\lambda^{-1}). \tag{13}$$

If we evaluate the coefficient of λ in this equation for the profile

$$\Phi(y) = \tanh(y) \tag{14}$$

we find the coefficient has the value of $1/3\pi \approx 0.106$. This is smaller than the exact value of the coefficient for the tanh profile [3] which is $3(2-\zeta(2))/2\pi \approx 0.170$.

It follows then that the approximation for $(E-E_0)/\Delta_0$ given in equation (11) is quantitatively correct for small λ and qualitatively correct for large λ.

We have numerically integrated equation (6) for the tanh soliton profile and determined λ_{approx} the value of λ that minimizes the approximate soliton creation energy. We find that

$$\lambda_{\text{approx}} \approx 0.82 \qquad (E-E_0)^{\text{approx}}/\Delta_0 \approx 1.083(2/\pi) \tag{15a}$$

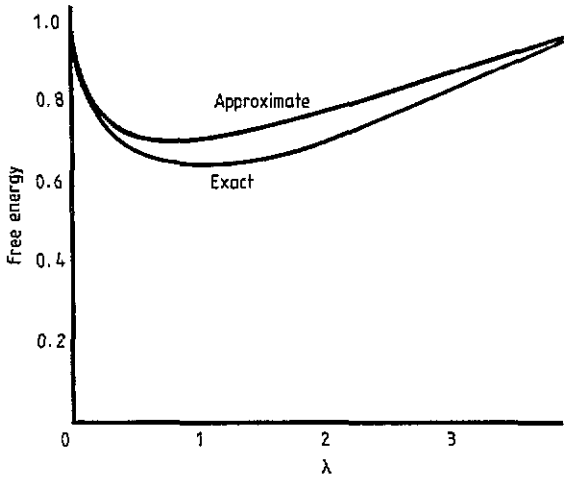

Figure 1. The approximate soliton creation energy $(E-E_0)^{\text{approx}}/\Delta_0$ and the exact soliton creation energy $(E-E_0)/\Delta_0$ are plotted as functions of the size parameter λ. In both the exact and approximate soliton creation energies a hyperbolic tangent soliton profile was used.

and these are to be compared with the exact results

$$\lambda = 1 \qquad (E-E_0)/\Delta_0 = 2/\pi. \tag{15b}$$

In figure 1 we present plots of $(E-E_0)^{\text{approx}}/\Delta_0$ and $(E-E_0)/\Delta_0$ for λ in the range 0 to 4. Given the essential simplicity of the approximation there is a remarkable correspondence between the exact and approximate results.

Let us summarize what has been done. The free energy has been approximated by the term quadratic in the potential along with an additive constant. We have found that at zero temperature there is a good qualitative and quantitiative agreement with the exact free energy. It should be emphasized that we have not performed a systematic expansion, in contrast to [1] and [3]; there is nothing particularly small about the potential V at zero temperature. Indeed one may well suspect that the results we have obtained would only follow from a non-systematic expansion that is able to encapsulate widely differing behaviours.

Acknowledgments

This work has received support from the Royal Society, the Science and Engineering Research Council (UK) and a Grant-In-Aid for Science Research from the Ministry of Education, Japan. One of us (DW) would like to thank the Department of Physics in the Faculty of Liberal Arts of Shizuoka University for their hospitality during his visit there.

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