Reply to "Comment on 'Thermodynamics of quantum crystalline membranes'"

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We reply to the preceding Comment by Kats and Lebedev [Phys. Rev. B **90**, 176301 (2014)] about our paper [Phys. Rev. B **89**, 224307 (2014)]. Kats and Lebedev criticize the validity of our calculation with the use of a Debye momentum as an ultraviolet regulator of the theory and the obtention of a k^2 term for the self-energy of out-of-plane modes. The arguments presented by Kats and Lebedev ignore basic facts about the theory of crystalline membranes. We address and counter argue the criticisms presented about our paper.

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In their Comment [1], Kats and Lebedev criticize the results obtained in our paper Ref. [2]. The main criticism by Kats and Lebedev [1] concerns the obtention of a k^2 term (k is the momentum) for the self-energy of the out-of-plane mode of a flat quantum crystalline membrane. In our paper, we found out that this k^2 has its origin in high-momentum modes. Kats and Lebedev [1] argue that in a continuum theory such high-momentum contributions cannot be rigorously estimated and, identifying the k^2 term as a tension, claim that such a term has to be set to zero.

Kats and Lebedev suggest in their Comment [1] that such a cancellation has to be performed by adding an extra term to the original action of the form $(\partial h)^2$ such that the contribution proportional to k^2 of the self-energy is exactly zero. Although such a procedure could be followed, we disagree with it.

First of all, in condensed matter, continuum field theories arise as long-wavelength approximations to a more fundamental and complete theory that is usually known. Long-wavelength continuous field theories are useful in order to study effects which would be computationally intractable if one were to use the complete theory, such as an atomistic model or an *ab initio* method. In this situation, the parameters to be used in the bare action of the field theory are to be fed from results from the more complete theory, solved in a certain approximation which does not capture the effect we wish to study with the field theory. While using the field theory, one will generally be faced with divergent contributions due to high momentum. This just means that modes with all momenta (modes over all the Brillouin zone) will contribute to a given quantity. Although the field theory is, strictly speaking, not valid at high momenta, the contribution from high-momentum modes can be estimated using a high-momentum cutoff on the order of $\sim 1/a$, the Debye momentum. A paradigmatic example of such an approach is the Debye model for the specific heat of solids. This is the approach we follow in our paper Ref. [2]. For the bare parameters of our model, we use values obtained using an atomistic classical model [3,4]. Then, we use a continuous field theory in order to study the effects of quantum fluctuations (which are not taken into account in the classical model) and long-wavelength fluctuations in the thermodynamic limit (the atomistic model is limited to study finite-size systems). The atomistic model does not predict a term of the form $(\partial h)^2$ for the bare action used in our model, and therefore we do not see why such a term should be included.

Second, we point out that in order to obtain an exact cancellation of the k^2 term in the self-energy, the coefficient of $(\partial h)^2$ to be added to the bare action would have to be finely tuned. Such tuning is unnatural. It is true that in some circumstances one can be interested in studying such a fine-tuned system as is the case when a ϕ^4 theory is used to describe the critical point of a phase transition and we have to adjust the parameters of the bare action such that the physical mass of the ϕ field is zero. However, for a phase transition there exists a parameter that can naturally be tuned in order to have a zero mass: the temperature. For a free crystalline membrane (no externally applied tensions) at zero temperature, there are no such parameters that we can tune in order to set the k^2 term of the self-energy to zero. The tuning of the coefficient of $(\partial h)^2$ is even more unnatural if we expect the continuous field theory to be able to describe different kinds of membranes, such as graphene, boron nitride, or transition-metal dichalcogenide monolayers.

Most importantly, Kats and Lebedev [1] seem to ignore some basic facts regarding the physics of classical crystalline membranes. Starting from the phenomenological dispersion relation for out-of-plane modes,

$$\rho\omega^2 = \sigma k^2 + \kappa k^4 \tag{1}$$

(where ρ is the mass density, σ is an external tension, and κ is the bending rigidity), Kats and Lebedev [1] identify the k^2 term obtained by us in Ref. [2] as a tension. What Kats and Lebedev [1] ignore is that relation (1) is only valid at the mean-field level and that inclusion of fluctuations leads to a radical reconstruction of the dispersion relation. It is very well known that at the classical level thermal fluctuations lead to an anomalous dependence of the out-of-plane displacement correlation function on momentum $\langle h_k h_{-k}\rangle \sim k^{\eta-4}$ (where $\eta > 0$ is an anomalous exponent) [5,6]. For a strained membrane, this anomalous dependence on momentum of the correlation function still occurs, provided the external tension is small enough [7]. In this situation Eq. (1) is no longer valid

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but would have to be replaced by

$$\omega^2 = \sigma k^2 + \kappa_R(k) k^4, \tag{2}$$

where $\kappa_R(k) = \kappa + \Sigma_k / k^4$ is a renormalized bending rigidity, which for $k \to 0$ behaves as $\kappa_R(k) \sim k^{-\eta}$. For a free membrane, $\sigma = 0$, and to first order in perturbation theory the self-energy is given by [5,6]

$$\begin{aligned}\Sigma_k &= \frac{4\mu(\lambda+\mu)}{\lambda+2\mu} k_B T \int \frac{d^2q}{(2\pi)^2} \frac{[\vec{k}\times\vec{q}]^4}{q^4} \frac{1}{\kappa|\vec{k}+\vec{q}|^2} \\ &= \frac{4\mu(\lambda+\mu)}{\lambda+2\mu} \frac{3k_B T}{16\pi\kappa} k^2. \end{aligned} \tag{3}$$

Therefore, to lowest order in perturbation theory we obtain the k^2 term in the dispersion relation for the out-of-plane mode. Notice that this result is obtained in the classical theory of crystalline membranes without employing any kind of regularization. This is a well-known result, which has been used to estimate the momentum scale below (or, with the replacement $k \to 2\pi/L$, the membrane size above) which anharmonic effects become dominant (see, for instance, Eq. (11) from Ref. [5], Eq. (5.2) from Ref. [8], Eq. (10) from Ref. [9], and Eq. (40) of Ref. [10]). Nobody involved with the theory of membranes has ever claimed, to our knowledge, that this term should be just neglected, in virtue of the condition of zero surface tension. At $T = 0$, the term we have found in first order in perturbation theory has the same k^2 dependence.

Furthermore, the contribution of the out-of-plane mode for the specific heat of the membrane at zero external stress only behaves as T^2 at the mean-field level with the dispersion relation Eq. (1). If the dispersion relation of the out-of-plane mode is altered, either by thermal fluctuations at high temperatures or by quantum fluctuations at low temperatures, then the T^2 behavior no longer holds as stated in our paper.

In conclusion, we insist that the k^2 term in the self-energy of the out-of-plane mode is not a tension term but a correction to the momentum dependence of the out-of-plane correlation function of a free membrane. A similar k^2 term is also found at the same perturbative level in the classical theory of membranes [5]. Therefore, we do not see why such a term should be forced to be zero by adding an extra term to the bare action, which would have to be finely tuned in order for the cancellation to take place. Furthermore, the use of a high-momentum cutoff and its identification with the Debye momentum allows us to estimate the contribution from high-momentum modes and is enough to make the kind of estimations we perform in our paper Ref. [2]. Therefore, we consider the criticisms made by Kats and Lebedev [1] to be unjustified.

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