Lowest Landau level approximation in strongly type-II superconductors

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Higher than the lowest Landau level, (LLL) contributions to magnetization and specific heat of superconductors are calculated using the Ginzburg-Landau equation approach. Corrections to the excitation spectrum around the solution of these equations (treated perturbatively) are found. Due to symmetries of the problem leading to numerous cancellations the range of validity of the LLL approximation in the mean field is much wider then a naive range and extends all the way down to $H = H_{c2}(T)/13$. Moreover, the contribution of higher Landau levels (HLL) is significantly smaller compared to LLL than expected naively. Like the LLL part, the lattice excitation spectrum at small quasimomenta is softer than that of the usual acoustic phonons. This enhances the effect of fluctuations. The mean-field calculation extends to third order, while the fluctuation contribution due to HLL is to one loop. This complements the earlier calculation of the LLL part to two-loop order. [S0163-1829(99)03834-5]

I. INTRODUCTION

The Ginzburg-Landau (GL) effective description of high- T_c superconductors has been remarkably successful in describing various thermodynamical and transport properties.¹ However, when fluctuations are of importance, even this effective description becomes very complicated. Some progress can be achieved when certain additional assumptions are made. One often made additional assumption is that only the lowest Landau level (LLL) significantly contributes to physical quantities of interest.^{2–8} There is a debate, however, on how restrictive the LLL approximation actually is. Naively when $H < H_{c2}(T)/3$ (see the dotted line in Fig. 1), even within the mean-field approximation, one should consider higher Landau levels (HLL's) mixing in the Abrikosov vortex lattice solution of the GL equations. When fluctuations are included one can argue using Hartree approximation μ ⁹ that the LLL range of validity is even smaller. However, direct application of the LLL scaling to magnetization and specific heat on Y-Ba-Cu-O suggest that the range of applicability is much wider—all the way down to $1-3T$.^{10,7,11} It is not clear why HLL do not contribute.

In this paper we explicitly calculate the effects of HLL at low temperatures in the vortex solid or liquid phase and establish the realistic range where the LLL approximation is valid (see the heavy dashed line in Fig. 1). We reanalyze the HLL corrections to mean-field equations going to higher order than in Ref. 12 and find that the expansion converges for H_{c2} $>$ *H* $>$ *H_c* $>$ /13. Importantly, within this radius of convergence the LLL contribution constitutes more than 95%. Then we calculate the HLL fluctuation effects to one-loop order complementing the LLL calculation to two loops by one of $us⁸$ (later referred to as I).

Ginzburg parameter *Gi* characterizing the importance of thermal fluctuations is much larger in high- T_c superconductors then in the low-temperature ones. Moreover, in the presence of the magnetic field the importance of fluctuations in high- T_c superconductors is further enhanced. Under these circumstances corrections to various physical quantities like magnetization or specific heat are not negligible even at low temperatures. It is quite straightforward to systematically ac-

FIG. 1. The range of the validity of the expansions in a_h and the loop expansion. The region above the dotted line is the naively expected validity range of the LLL approximation. The region above the long dashed line is the actual validity range for the expansion of the mean-field equations. The loop expansion applicability range lies below the dashed curves. We plot two curves with different values of Ginzburg number Gi , $Gi = 0.1$, and $Gi = 0.01$. The validity combining the mean-field expansion and the loop expansion lies therefore between the long dashed line and the dashed curves.

count for the fluctuations effect on magnetization, specific heat or conductivity perturbatively above the mean-field transition line using the Ginzburg-Landau description.¹³ However, in the interesting region below this line it turned out to be extremely difficult to develop a quantitative theory.

Within LLL in order to approach the region below the mean-field transition line $T < T_{mf}(H)$, Thouless² proposed a perturbative approach around the homogeneous (liquid) state was in which all the ''bubble'' diagrams are resumed. The series provide accurate results at high temperatures, but for the LLL dimensionless temperature a_T $\equiv (2H_{c2}^2/GiT_cT^2H^2)^{1/3}[T-T_{mf}(H)/\pi] \leq -2$ become inapplicable. Generally attempts to extend the theory to lower temperature by Padé extrapolation were not successful.⁴ Alternatively, a more direct approach to low-temperature fluctuations physics is to start from the mean field solution and then take into account perturbative fluctuation around this inhomogeneous solution. Experimentally it is reasonable since, for example, specific heat at low temperatures is a smooth function and the fluctuation contribution experimentally is quite small. For some time this was in disagreement with theoretical expectations.

Eilenberger calculated the spectrum of harmonic excitations of the triangular vortex lattice [see Eq. (30) below]³ and noted that the gapless mode is softer then the usual Goldstone mode expected as a result of the spontaneous breaking of translational invariance. The inverse propagator for the "phase" excitations behaves as $k_z^2 + \text{const}(k_x^2 + k_y^2)^2$. The influence of this unexpected additional "softness" apparently goes beyond the enhancement of the contribution of fluctuations at leading order. It leads to disastrous infrared divergences at higher orders rendering the perturbation theory around the vortex state doubtful. One, therefore, tends to think that nonperturbative effects are so important that such a perturbation theory should be abandoned.¹⁴ However, it was shown in I that a closer look at the diagrams reveals that in fact one encounters actually only logarithmic divergences. This makes the divergences similar to so-called ''spurious'' divergences in the theory of critical phenomena with broken continuous symmetry and they exactly cancel out each other, provided we are calculating a symmetric quantity. Qualitatively physics of a fluctuating $D=3$ GL model in a magnetic field turns out to be similar to that of spin systems in $D=2$ possessing a continuous symmetry. In particular, although within perturbation theory in the thermodynamic limit the ordered phase (solid) exists only at $T=0$, at low temperatures liquid differs very little in most aspects from solid. One can effectively use properly modified perturbation theory to quantitatively study various properties of the vortex-liquid phase. This perturbative approach agrees very well with the direct Monte Carlo simulation of Ref. 7. The question arises whether one can extend the well-controlled perturbative calculation beyond the LLL. Sometimes a hope is expressed that the additional softness is an accidental artifact of LLL approximation. We will show that this is not so and it is a fundamental general phenomenon (see also Ref. 15).

The paper is organized as follows. The model is described and a perturbative mean-field solution is developed in Sec. II. The expansion parameter will be the distance from the mean-field critical line $a_h \equiv \frac{1}{2} (1 - T/T_c - H/H_{c2})$. The range of validity of the expansion and of the LLL approximation is discussed. Then in Sec. III we derive the spectrum of excitations to leading order and to the next to leading order in *ah* . The free energy to one loop is calculated in Sec. IV. Section V contains expressions for magnetization and specific heat and a discussion of the validity range of the fluctuation contributions calculation. Finally, we summarize the results in Sec. VI. Details of the mean-field calculation can be found in Appendix A, while details of the HLL spectrum calculation can be found in Appendix B.

II. MODEL AND THE PERTURBATIVE MEAN-FIELD SOLUTION

A. Model

Our starting point is the GL free energy:

$$
F = \int d^3x \frac{\hbar^2}{2m_{ab}} \left| \left(\vec{\nabla} - \frac{ie^*}{\hbar c} \vec{A} \right) \psi \right|^2 + \frac{\hbar^2}{2m_c} |\partial_z \psi|^2 + a |\psi|^2
$$

+
$$
\frac{b'}{2} |\psi|^4.
$$
 (1)

Here $A = (By,0)$ describes a nonfluctuating constant magnetic field. For strongly type-II superconductors ($\kappa \sim 100$) far from H_{c1} (this is the range of interest in this paper) the magnetic field is homogeneous to a high degree due to superposition from many vortices. For simplicity we assume $a = \alpha(1-t)T_c$, $t \equiv T/T_c$, although this dependence can be easily modified to better describe the experimental coherence length.

Throughout most of the paper will use the following units. The unit of length is $\xi = \sqrt{\hbar^2/(2m_{ab}\alpha T_c)}$ and the unit of the magnetic field is H_{c2} , so that the dimensionless magnetic field is $b = B/H_{c2}$. The dimensionless Boltzmann factor in these units is [the order parameter field is rescaled as ψ^2 \rightarrow (2 $\alpha T_c/b')\psi^2$:

$$
\frac{F}{T} = \frac{1}{\omega} \int d^3 x \frac{1}{2} |D \psi|^2 + \frac{1}{2} |\partial_z \psi|^2 - \frac{1 - t}{2} |\psi|^2 + \frac{1}{2} |\psi|^4.
$$
\n(2)

The dimensionless coefficient is

$$
\omega = \sqrt{2Gi} \pi^2 t,\tag{3}
$$

where the Ginzburg number is defined by *Gi* $\equiv \frac{1}{2} (32\pi e^2 \kappa^2 \xi T_c \gamma^{1/2} / c^2 h^2)^2$ and $\gamma = m_c / m_{ab}$ is an anisotropy parameter. This coefficient determines the strength of fluctuations, but is irrelevant as far as mean-field solutions are concerned.

B. Mean-field solution by expansion in *ah*

Now we turn to a perturbative solution of the Ginzburg-Landau equations near the mixed-state–normal-phase transition line. This has been done before¹² to second order, however, the range of applicability and precision of the LLL approximation at large κ has not been fully explored. The *z* direction dependence of the solutions is trivial and will not be mentioned until fluctuations will be discussed. The expansion parameter is

$$
a_h \equiv \frac{1 - t - b}{2}.
$$
 (4)

Rewriting the quadratic part in terms of operator ("Hamiltonian'') $\mathcal{H} = \frac{1}{2}(-D^2 - b)$ whose spectrum starts from zero, one obtains the following free-energy density over *T*

$$
\frac{F}{T} = \frac{f}{\omega} = \frac{1}{\omega} \int d^2x \left(\psi^* \mathcal{H} \psi - a_h |\psi|^2 + \frac{1}{2} |\psi|^4 \right). \tag{5}
$$

The equation of motion is therefore

$$
\mathcal{H}\psi - a_h\psi + \psi|\psi|^2 = 0.
$$
 (6)

This equation is solved perturbatively in *ah* by assuming

$$
\Phi = (a_h)^{1/2} [\Phi_0 + a_h \Phi_1 + \cdots].
$$
 (7)

It is convenient to represent Φ_0, Φ_1, \ldots in the basis of eigenfunctions of H , $H\varphi^{n} = nb\varphi^{n}$, normalized to unit "Cooper pairs density" $\langle |\varphi^n|^2 \rangle = \int_{\text{cell}} d^2x |\varphi^n|^2 b/2\pi = 1$, where "cell" is a primitive cell of the vortex lattice. Assuming hexagonal lattice symmetry one explicitly has

$$
\varphi^{n} = \sqrt{\frac{2\pi}{\sqrt{\pi}2^{n}n!a}} \sum_{l=-\infty}^{\infty} H_{n} \left(y\sqrt{b} - \frac{2\pi}{a}l \right) \exp\left\{ i \left[\frac{\pi l(l-1)}{2} + \frac{2\pi\sqrt{b}}{a}l x \right] - \frac{1}{2} \left(y\sqrt{b} - \frac{2\pi}{a}l \right)^{2} \right\},
$$
\n(8)

where $a/\sqrt{b} = \sqrt{4\pi/\sqrt{3}b}$ is the lattice spacing. To order zero

$$
\mathcal{H}\Phi_0=0,\tag{9}
$$

and Φ_0 is proportional to the Abrikosov vortex lattice solution φ which is Eq. (6) for $n=0$:

$$
\Phi_0 = g_0 \varphi.
$$

To order *k*, one expands

$$
\Phi_i = g_i \varphi + \sum_{n=1}^{\infty} g_i^n \varphi^n.
$$
\n(10)

Inserting into Eq. (6), one obtains to order a_h^3 :

$$
\mathcal{H}\Phi_1 = g_0\varphi - g_0|g_0|^2\varphi|\varphi|^2. \tag{11}
$$

Taking the inner product with φ one finds that

$$
g_0 = \frac{1}{\sqrt{\beta_A}},\tag{12}
$$

where the Abrikosov's constant is the following average over the primitive cell: $\beta = \beta_A = \langle |\varphi|^4 \rangle \approx 1.16$. Inner product with φ^n determines g_1^n :

$$
g_{1,n} = -\frac{\beta^n}{nb\beta^{3/2}},\tag{13}
$$

where $\beta^n \equiv \langle |\varphi|^2 \varphi^n \varphi^* \rangle$. To find g_1 we need in addition also the order $a_h^{5/2}$ equation:

$$
\mathcal{H}\Phi_2 = \Phi_1 - (g_0)^2 (2\Phi_1|\varphi|^2 + \Phi_1^* \varphi^2). \tag{14}
$$

The inner product with φ gives

$$
g_1 = \frac{3}{2} \sum_{n=1}^{\infty} \frac{(\beta^n)^2}{nb \beta^{5/2}}.
$$
 (15)

C. Mean-field result for free energy: Orders a_h^2 and a_h^3

The mean-field expression for the free energy to order $a_h²$ is well known. Inserting the next correction Eq. (7) into Eq. (5) one obtains the free-energy density:

$$
\frac{\mathcal{F}_{\text{mf}}}{T} = \frac{1}{\omega} \left[-\frac{a_h^2}{2\beta} - \frac{a_h^3}{\beta^3 b} \sum_{n=1}^{\infty} \frac{(\beta^n)^2}{n} \right]
$$

$$
= \frac{1}{\omega} \left[-0.43a_h^2 - 0.0078 \frac{a_h^3}{b} \right].
$$
(16)

It is interesting to note that $\beta_n \neq 0$ only when $n=6j$, where j is an integer. This is due to the hexagonal symmetry of the vortex lattice.¹² For $n=6j$ it decreases very fast with *j*: $\beta_6 = -0.2787, \beta_{12} = 0.0249$. Because of this the coefficient of the next-to-leading order is very small (additional factor of 6 in the denominator). We might preliminarily conclude therefore that the perturbation theory in a_h works much better than might be naively anticipated (see dashed line on Fig. 1) and can be used very far from transition line. If we demand that the correction is smaller then the main contribution, the corresponding line on the phase diagram will be $b=0.015\times(1-t)$. For example, the LLL melting line corresponds to $a_h \sim 1$. This overly optimistic conclusion is, however, incorrect as the calculation of the following term in Appendix A shows.

D. Range of applicability of the expansion. How precise is LLL?

Now we discuss in what region of the parameter space the expansion outlined above can be applied. First of all note that all the contributions to Φ_1 are proportional to $1/b$. This is a general feature: the actual expansion parameter is a_h/b . One can check as to whether the expansion is convergent and, if yes, what is its radius of convergence. Looking just at the leading correction and comparing it to the LLL one gets a very optimistic estimate. For this purpose we calculated higher-order coefficients in Appendix A. The results for the Φ_2 are the following:

 $g_2^n = \frac{1}{nb}$ $g_1^n - \frac{1}{\beta} \sum_{i=0}^\infty$ ∞ $g_1^i(2\langle n,0|i,0\rangle + \langle 0,0|i,n\rangle)$ (17)

and

$$
g_2 = -\frac{3}{2\beta}\beta^n g_2^n - \frac{1}{2\sqrt{\beta}} \sum_{i,j=0}^{\infty} g_1^i g_1^j(\langle 0,0 | i,j \rangle + 2\langle j,0 | i,0 \rangle), \tag{18}
$$

where $\langle i_1, i_2 | j_1, j_2 \rangle \equiv \langle \varphi^{*i_1} \varphi^{*i_2} \varphi^{j_1} \varphi^{j_2} \rangle$ and g_j^i when $i=0$ is defined to be equal to g_j , $\varphi^i = \varphi$ when $i = 0$.

We already can see that g_2^n and g_2 are proportional to g_1^n and in addition there is a factor of 1/*n*. Since, due to hexagonal lattice symmetry all the g_1^n , $n \neq 6j$ vanish, so do g_2^n . We

FIG. 2. The density $|\psi^2|$ of the mean-field Abrikosov solution for $b=0.1$, $t=0.5$. (a) is the lowest order approximation (LLL). (b) is the solution with the next-order correction included, while in (c) the next-next-order correction is included.

checked that there is no more small parameters, so we conclude that the leading-order coefficient is much larger than the first (factor 6×5), but the second is only 6 times larger than the third.

The correction to free energy is

$$
\frac{\mathcal{F}_{\rm mf}}{T} = \frac{1}{\omega} \cdot \frac{0.056}{6^2} \frac{a_h^4}{b^2}.
$$
\n(19)

Accidental smallness by a factor of 1/6 of the coefficients in the a_h/b expansion due to symmetry means that the range of validity of this expansion is roughly $a_h < 6b$ or $H < H_{c2}/13$. Moreover, additional smallness of all the HLL corrections compared to the LLL means that they constitute just several percent of the correct result inside the region of applicability. To illustrate this point we plot in Fig. 2 the perturbatively calculated solution for $b=0.1, t=0.5$. One can see that although the leading LLL function has very thick vortices [Fig. $2(a)$, the first nonzero correction makes them of the order of the coherence length [Fig. 2(b)]. Following the correction of the order $(a_h/b)^2$ makes it practically indistinguishable from the numerical solution. Amazingly the order parameter between the vortices approaches its vacuum value. Paradoxically starting from the region close to H_{c2} the perturbation theory knows to correct the order parameter so that it looks very similar to the London approximation (valid only close to H_{c1}) result of well-separated vortices.

We conclude, therefore, that the expansion in a_h/b works in the mean field better than one can naively expect. In the next section we investigate whether the same is true for the fluctuation contribution.

III. FLUCTUATIONS SPECTRUM

A. Fluctuations to leading order in *a*

To find an excitation spectrum in the harmonic approximation one expands the free-energy functional around the solution found in the previous section. Within the LLL approximation this has been done in Ref. 3. We generalize it to the case of all the Landau levels when perturbations due to nonlinear term are included. The fluctuating order-parameter field ψ should be divided into a nonfluctuating (mean field) part and a small fluctuation

$$
\psi(x) = \Phi(x) + \chi(x). \tag{20}
$$

The energy Eq. (5) is then expanded in χ retaining only quadratic terms

$$
f_2 = \int d^2x \left[\chi^* \mathcal{H} \chi - a_h |\chi|^2 + 2 |\Phi|^2 |\chi|^2 + \frac{1}{2} (\Phi^{*2} \chi^2 + \Phi^2 \chi^{*2}) \right].
$$
 (21)

Field χ can be expanded in a basis of quasimomentum \overline{k} eigenfunctions:

$$
\varphi_{\vec{k}}^n = \sqrt{\frac{2\pi}{\sqrt{\pi}2^n n! a}} \sum_{l=-\infty}^{\infty} H_n \left(y \sqrt{b} + \frac{k_x}{\sqrt{b}} - \frac{2\pi}{a} l \right)
$$

$$
\times \exp \left\{ i \left[\frac{\pi l (l-1)}{2} + \frac{2\pi \left(\sqrt{b} x - \frac{k_y}{\sqrt{b}} \right)}{a} l - x k_x \right] - \frac{1}{2} \left(y \sqrt{b} + \frac{k_x}{\sqrt{b}} - \frac{2\pi}{a} l \right)^2 \right\}.
$$
(22)

In addition instead of complex field χ_k^n we will use two "real" fields O_k^n and A_k^n satisfying $O_k^n = O_{-k}^{*n}$, $A_k^n = A_{-k}^{*n}$.

$$
\chi(x) = \int_{\vec{k}, n=0}^{\infty} \varphi_{\vec{k}}^{n}(x) (O_{k}^{n} + iA_{k}^{n}),
$$
 (23)

$$
\chi^*(x) = \int_{\vec{k}, n=0}^{\infty} \varphi_{\vec{k}}^{*n}(x) (O_{-k}^n - iA_{-k}^n).
$$

In terms of these fields representing ''optical'' and ''acoustic'' phonons Eq. (21) takes a form

$$
f_2 = \int_{\vec{k}, n=1}^{\infty} (nh - a_h)(O_k^n O_{-k}^n + A_k^n A_{-k}^n)
$$

\n
$$
-a_h(O_k O_{-k} + A_k A_{-k})
$$

\n
$$
+ \sum_{i,j=0}^{\infty} A_k^i A_{-k}^j K_k^{i,j} + O_k^i A_{-k}^j L_k^{i,j}
$$

\n
$$
+ O_{-k}^i A_k^j M_k^{i,j} + O_k^i O_{-k}^j N_k^{i,j}
$$

where elements of the matrix are

$$
K_{k}^{i,j} = \left\langle |\Phi|^{2} (\varphi_{-\vec{k}}^{*i} \varphi_{-\vec{k}}^{j} + \varphi_{\vec{k}}^{i} \varphi_{\vec{k}}^{*j}) - \frac{1}{2} (\Phi^{*2} \varphi_{\vec{k}}^{i} \varphi_{-\vec{k}}^{j} + \Phi^{2} \varphi_{-\vec{k}}^{*i} \varphi_{\vec{k}}^{*j}) \right\rangle,
$$

$$
N_{k}^{i,j} = \left\langle |\Phi|^{2} (\varphi_{-\vec{k}}^{*i} \varphi_{-\vec{k}}^{j} + \varphi_{\vec{k}}^{i} \varphi_{\vec{k}}^{*j}) - \frac{1}{2} |\Phi|^{2} (\varphi_{-\vec{k}}^{*i} \varphi_{-\vec{k}}^{j} + \varphi_{\vec{k}}^{i} \varphi_{\vec{k}}^{*j}) \right\rangle,
$$

$$
+\frac{1}{2}(\Phi^{*2}\varphi_{\vec{k}}^{i}\varphi_{-\vec{k}}^{j}+\Phi^{2}\varphi_{-\vec{k}}^{*i}\varphi_{\vec{k}}^{*j})\bigg\rangle, \qquad (25)
$$

$$
L_k^{i,j} = i \left\langle |\Phi|^2 (\varphi_{-\vec{k}}^{*i} \varphi_{-\vec{k}}^j - \varphi_{\vec{k}}^i \varphi_{\vec{k}}^{*j}) + \frac{1}{2} (\Phi^{*2} \varphi_{\vec{k}}^i \varphi_{-\vec{k}}^j - \Phi^2 \varphi_{-\vec{k}}^{*i} \varphi_{\vec{k}}^{*j}) \right\rangle,
$$

$$
M_{k}^{i,j} = -i \left\langle |\Phi|^2 (\varphi_{-\vec{k}}^{*i} \varphi_{-\vec{k}}^j - \varphi_{\vec{k}}^i \varphi_{\vec{k}}^{*j}) + \frac{1}{2} (\Phi^{*2} \varphi_{\vec{k}}^i \varphi_{-\vec{k}}^j - \Phi^{2} \varphi_{-\vec{k}}^{*i} \varphi_{\vec{k}}^{*j}) \right\rangle.
$$

We expand f_2 in a_h . The order a_h term is

$$
\int_{\vec{k}.i=0}^{\infty} -a_h (O_k^i O_{-k}^i + A_k^i A_{-k}^i) + a_h \sum_{i,j}^{\infty} [A_k^i A_{-k}^j K_k^{i,j}(1) + O_k^i A_{-k}^j L_k^{i,j}(1) + O_{-k}^i A_k^j M_k^{i,j}(1) + O_k^i O_{-k}^j N_k^{i,j}(1)].
$$
\n(26)

We will use the degenerate perturbation theory similar to one used in quantum mechanics to calculate the correction to the eigenvalues of the matrix the LLL states $(A, O \text{ states})$ to order a_h^2 . The matrix $\hat{H} = \begin{pmatrix} K & L \\ M & N \end{pmatrix}$ is analogous to the "Hamiltonian," while (A/O) is analogous to the eigenvector. Explicitly the matrix elements are

$$
K_{k}^{i,j}(1) = \frac{1}{\beta} \left\{ |\varphi|^{2} (\varphi_{-\vec{k}}^{*i} \varphi_{-\vec{k}}^{j} + \varphi_{\vec{k}}^{i} \varphi_{\vec{k}}^{*j}) - \frac{1}{2} (\varphi^{*2} \varphi_{\vec{k}}^{i} \varphi_{-\vec{k}}^{j} + \varphi^{2} \varphi_{-\vec{k}}^{*i} \varphi_{\vec{k}}^{*j}) \right\},
$$

$$
N_{k}^{i,j}(1) = \frac{1}{\beta} \left\{ |\varphi|^{2} (\varphi_{-\vec{k}}^{*i} \varphi_{-\vec{k}}^{j} + \varphi_{\vec{k}}^{i} \varphi_{\vec{k}}^{*j}) + \frac{1}{2} (\varphi^{*2} \varphi_{\vec{k}}^{i} \varphi_{-\vec{k}}^{j} + \varphi^{2} \varphi_{-\vec{k}}^{*i} \varphi_{\vec{k}}^{*j}) \right\},
$$
(27)

$$
L_{k}^{i,j}(1) = \frac{1}{\beta} \left(|\varphi|^{2} (\varphi_{-\vec{k}}^{*i} \varphi_{-\vec{k}}^{j} - \varphi_{\vec{k}}^{i} \varphi_{\vec{k}}^{*j}) \right)
$$

 $\frac{1}{2}(\,\varphi^{\ast\,2}\varphi^i_{\vec{k}}\varphi^j_{-\vec{k}}\!-\!\varphi^2\varphi^{\ast i}_{-\vec{k}}\varphi^{\ast j}_{\vec{k}})\bigg\rangle,$

$$
M_{k}^{i,j}(1) = \frac{1}{\beta} \left\{ |\varphi|^2 (\varphi_{-\vec{k}}^{*i} \varphi_{-\vec{k}}^j - \varphi_{\vec{k}}^i \varphi_{\vec{k}}^{*j}) + \frac{1}{2} (\varphi^{*2} \varphi_{\vec{k}}^i \varphi_{-\vec{k}}^j - \varphi^2 \varphi_{-\vec{k}}^{*i} \varphi_{\vec{k}}^{*j}) \right\}.
$$

We will use definitions

 $^{+}$

$$
\beta_k^n = \langle |\varphi|^2 \varphi_k \varphi_k^{*n} \rangle,
$$

$$
\overline{\beta_k^n} = \langle \varphi^* \varphi^n \varphi_k^* \varphi_k \rangle,
$$

$$
\gamma_k^n = \langle (\varphi^*)^2 \varphi_{-\vec{k}} \varphi_k^n \rangle,
$$

$$
\overline{\gamma_k^n} = \langle \varphi^* \varphi^{*n} \varphi_k \varphi_{-\vec{k}} \rangle.
$$
 (28)

When an index is zero we drop it throughout the paper. For example, when $n=0$, we refer to β_k^n as β_k , and when *k* $=0, \beta_k^n = \beta^n$, etc.).

Considering to order a_h above matrix element $i, j = 0$ of *K*,*L*,*M*,*N* is

$$
K_1 = \frac{2}{\beta} \beta_k - \frac{1}{\beta} \text{Re } \gamma_k,
$$

$$
N_1 = \frac{2}{\beta} \beta_k + \frac{1}{\beta} \text{Re } \gamma_k
$$
 (29)

$$
L_1 = M_k = -\frac{1}{\beta} \operatorname{Im} \gamma_k.
$$

In deriving this we have used a property $\beta_k = \beta_{-k}$.

We now diagonalize the matrix to find the eigenstates of LLL (which is of order a_h). Eigenvalues are

$$
\epsilon_A = a_h \bigg(-1 + \frac{2}{\beta} \beta_k - \frac{1}{\beta} |\gamma_k| \bigg), \tag{30}
$$

FIG. 3. The shear mode A spectrum. (a) is the spectrum obtained within the LLL approximation. (b) is the correction to the spectrum when the HLL mixing effect is considered.

$$
\epsilon_O = a_h \bigg(-1 + \frac{2}{\beta} \beta_k + \frac{1}{\beta} |\gamma_k| \bigg),
$$

as was found originally by Eilenberger.³ The "acoustic" branch is shown in Fig. $3(a)$. The rotation transforming in to these eigenstates is

$$
\widetilde{A}_k = \cos\frac{\theta_k}{2} A_k + \sin\frac{\theta_k}{2} O_k, \qquad (31)
$$

$$
\widetilde{O}_k = -\sin\frac{\theta_k}{2}A_k + \cos\frac{\theta_k}{2}O_k,
$$

where $\gamma_k = |\gamma_k| \exp[i\theta_k]$. A similar calculation for the *n*th Landau level gives the spectrum

$$
\varepsilon_{A,O}^{n} = a_{h} \bigg(-1 + \frac{2}{\beta} \langle |\varphi|^{2} \varphi_{k}^{*n} \varphi_{k}^{n} \rangle + \frac{1}{\beta} |\langle (\varphi^{*})^{2} \varphi_{k}^{n} \varphi_{-k}^{n} \rangle| \bigg). \tag{32}
$$

B. Spectrum of fluctuations beyond leading order in *ah*

In this subsection we calculate the correction of eigenvalues of LLL to order a_h^2 . The Hamiltonian \hat{H} in addition has the a_h part \hat{H}_1 given in Eq. (27) also has the a_h^2 part \hat{H}_2 . As will be explained in the next section, we will need only the correction to the LLL to the $a_h²$ order, not the HLL. Therefore we will need only the *i*, *j* = 0 matrix element of \hat{H}_2 :

$$
K_2 = \sum_{n=1}^{\infty} \frac{1}{nb\beta^2} \left[\frac{3}{\beta} \beta_n^2 (2\beta_k - \text{Re }\gamma_k) -2\beta_n (\text{Re }\bar{\beta}_k^n + \text{Re }\bar{\beta}_{-k}^n - \text{Re }\bar{\gamma}_k^n) \right],
$$

$$
N_2 = \sum_{n=1}^{\infty} \frac{1}{nb\beta^2} \left[\frac{3}{\beta} \beta_n^2 (2\beta_k + \text{Re }\gamma_k) -2\beta_n (\text{Re }\bar{\beta}_k^n + \text{Re }\bar{\beta}_{-k}^n + \text{Re }\bar{\gamma}_k^n) \right],
$$
 (33)

$$
L_2 + M_2 = \sum_{n=1}^{\infty} \frac{1}{nb\beta^2} \left[-\frac{6}{\beta} \beta_n^2 \operatorname{Im} \gamma_k + \frac{4}{\beta} \beta_n \operatorname{Im} \overline{\gamma}_k^n \right].
$$

Note that we do not show L_2 and M_2 separately as our result will depend only on $L_2 + M_2$. According to the degenerate perturbation theory we need to diagonalize \hat{H}_1 which already has been done in the previous subsection and then use the resulting states \tilde{A}_k and \tilde{O}_k to calculate the second-order correction to the eigenvalue: $\varepsilon_k^{(2)} = a_h^2 (E_{\text{diag}} + E_{\text{offdiag}})$. The diagonal contribution is

$$
E_{\text{diag}} = \langle \tilde{A}_k | \hat{H}_2 | \tilde{A}_k \rangle = \left(\cos \frac{\theta_k}{2} \right)^2 K_2 + N_2 \left(\sin \frac{\theta_k}{2} \right)^2
$$

$$
+ (L_2 + M_2) \sin \frac{\theta_k}{2} \cos \frac{\theta_k}{2}.
$$
(34)

Substituting the matrix elements Eq. (33) we obtain

bstituting the matrix elements Eq. (33) we obtain
\n
$$
E_{\text{diag}} = \sum_{n=1}^{\infty} \frac{\beta_n}{n b \beta^2} \left\{ \frac{3\beta_n}{\beta} (2\beta_k - |\gamma_k|) - 2[\text{Re } \overline{\beta_k^n} + \text{Re } \overline{\beta_{-k}^n}] - \cos \theta_k \text{ Re } \overline{\gamma_k^n} - \sin \theta_k \text{Im } \overline{\gamma_k^n}] \right\}.
$$
\n(35)

In the off-diagonal contribution

TABLE I. Contributions to the free energy of mixing the LLL with HLL. Given in units of $\frac{1}{2}\sigma b a_h^{3/2}$.

Level n					
A mode O mode	-0.253 -0.230	-0.082 -0.086	-0.053 -0.063 -0.063 0.247 -0.017 -0.051 -0.023 -0.012 0.018 -0.003		-0.005 -0.001

$$
E_{\text{offdiag}} = -\sum_{n=1}^{\infty} \frac{\langle \tilde{A}_k | \hat{H}_1 | n \rangle \langle n | \hat{H}_1 | \tilde{A}_k \rangle}{n b} = -\sum_{n} \frac{1}{n b} \left\{ \left(\cos \frac{\theta_k}{2} \right)^2 \left[|\langle A_k | \hat{H}_1 | A_k^n \rangle|^2 + |\langle A_k | \hat{H}_1 | O_k^n \rangle|^2 \right] + \left(\sin \frac{\theta_k}{2} \right)^2 \left[|\langle O_k | \hat{H}_1 | O_k^n \rangle|^2 \right] \right\}
$$

$$
+ |\langle O_k | \hat{H}_1 | A_k^n \rangle|^2 \left[+ \sin \frac{\theta_k}{2} \cos \frac{\theta_k}{2} \left[\langle A_k | \hat{H}_1 | A_k^n \rangle \langle A_k^n | \hat{H}_1 | O_k \rangle + \langle A_k | \hat{H}_1 | O_k^n \rangle \langle O_k^n | \hat{H}_1 | O_k \rangle + \text{c.c.} \right] \right]. \tag{36}
$$

Details of the calculation of these matrix elements can be found in Appendix B together with definitions of quantities *F*. The result is

$$
E_{\text{offdiag}} = -\frac{1}{b} \sum_{n} \frac{1}{n} \left\{ \frac{1}{\beta^2} \left[|F_{k}^{n}(1)|^2 + |F_{-k}^{n}(1)|^2 + |F_{k}^{n}(2)|^2 + |F_{-k}^{n}(2)|^2 + \frac{\cos \theta_k}{\beta^2} \left[|F_{k}^{n}(1)|^2 + |F_{-k}^{n}(1)|^2 - |F_{k}^{n}(2)|^2 \right] \right. \\ \left. - |F_{-k}^{n}(2)|^2 \right] + \frac{2 \sin \theta_k}{\beta^2} \text{Im} \left[F_{-k}^{n}(1) F_{-k}^{*n}(2) - F_{k}^{*n}(1) F_{k}^{n}(2) \right] \right\}.
$$
 (37)

A similar result for O_k can be obtained by changing the sign of cos θ_k and the sign of sin θ_k in the formula above.

It is crucial to see whether there is a k^2 term in higher orders for the acoustic branch *A*. We calculated numerically the contributions to the spectrum until $n=8$. All the k^2 contributions to any of them cancel, as it was proved in Ref. 15. Moreover even all the k^4 contributions for odd *n* cancel although the even *n* give a negative contribution to the rotationally symmetric combination $(k_x^2 + k_y^2)^2$. Numerically the coefficients are 2.2×10^{-6} , 5.0×10^{-5} , -6.3×10^{-6} , 4.7 $\times 10^{-7}$ for $n=2,4,6,8$ correspondingly. The resulting correction to the spectrum of the acoustic branch due to the $n=2$ level is shown in Fig. $3(b)$.

After we have established the spectrum of the elementary excitations of the Abrikosov lattice, we are ready to calculate the fluctuation contributions to various physical quantities.

IV. FLUCTUATION CONTRIBUTIONS TO FREE ENERGY, MAGNETIZATION AND SPECIFIC HEAT

Higher Landau levels contribution to free energy

The thermal fluctuation part is

$$
-T \ln[Z] = \mathcal{F}_{\text{mf}} + \mathcal{F}_{\text{fluc}};
$$

$$
\mathcal{F}_{\text{fluc}} = \frac{T}{2} \sum_{n=0}^{\infty} \left\{ \text{Tr} \ln \left[\varepsilon_A^n(k) + \frac{k_z^2}{2} \right] + \text{Tr} \ln \left[\varepsilon_O^n(k) + \frac{k_z^2}{2} \right] \right\}
$$
(38)

$$
= TL_{x}^{2}L_{z}\sigma b\sum_{n=0}^{\infty} \ [\langle\sqrt{\varepsilon_{A}^{n}(k)}\rangle + \langle\sqrt{\varepsilon_{O}^{n}(k)}\rangle],
$$

where $\sigma=1/\sqrt{2}2\pi$ and we performed the integration over k_z .

The LLL contribution to order $\sqrt{a_h}$ in two dimensions $(2D)$ has been calculated by Eilenberger.³ The 3D result for the density of the free energy is 8

$$
\frac{\mathcal{F}_{\text{fluc}}^{(1/2)}}{T} = \sigma b a_h^{1/2} [\langle \sqrt{\varepsilon_A^{(1)}(k)} \rangle + \langle \sqrt{\varepsilon_O^{(1)}(k)} \rangle] = 3.16 \sigma b a_h^{1/2}.
$$
\n(39)

We calculated its higher a_h correction which is of order $a_h^{3/2}$ using Eqs. (35) and (37)

$$
\frac{\mathcal{F}_{\text{fluc}}^{(3/2)}}{T} = \frac{1}{2} \sigma b a_h^{3/2} \left(\left\langle \frac{\varepsilon_A^{(2)}(k)}{\sqrt{\varepsilon_A^{(1)}(k)}} \right\rangle + \left\langle \frac{\varepsilon_O^{(2)}(k)}{\sqrt{\varepsilon_O^{(1)}(k)}} \right\rangle \right)
$$

$$
= -0.445 \sigma b a_h^{3/2} . \tag{40}
$$

As noted below $\varepsilon_A^{(2)}(k)$ and $\varepsilon_A^{(2)}(k)$ given in the last section contain contributions from mixing with all the HLL's. Table I details contributions to this term from levels until $n=8$. The contributions are negative for all $n \neq 6$ *j* where *j* is an integer and positive otherwise.

The contribution of HLL is

$$
\frac{\mathcal{F}_{\text{fluc}}}{T} = \sigma b \sum_{n=1}^{\infty} \left[\langle \sqrt{n b + a_h \varepsilon_A^n(k)} \rangle + \langle \sqrt{n b + a_h \varepsilon_O^n(k)} \rangle \right] \approx 2 \sigma b^{3/2} \sum_{n=1}^{\infty} \sqrt{n} + \frac{1}{2} \sigma b^{1/2} a_h \sum_{n=1}^{\infty} \frac{1}{\sqrt{n}} \left[\langle \varepsilon_A^n(k) \rangle + \langle \varepsilon_O^n(k) \rangle \right] + O(a_h^2)
$$
\n
$$
= \frac{1}{T} (\mathcal{F}_{\text{fluc}}^{(0)} + \mathcal{F}_{\text{fluc}}^{(1)}).
$$
\n(41)

The first divergent (as powers $3/2$ and $1/2$ in the ultraviolet) term renormalizes energy. However, it has a finite magneticfield-dependent part which should be calculated by subtracting the $b=0$ value of the free energy. The proper regularization is made by restricting the number of Landau levels and then showing that after regularization the answer does not depend on it. The calculation is the same as the one done in the normal phase (obviously uv divergences are insensitive to the phase in which they are calculated), see for details and discussion, Ref. 16. The result is

$$
\frac{\mathcal{F}_{\text{fluc}}^{(0)}}{T} = 0.526\sigma b^{3/2}.
$$
 (42)

This exhibits the diamagnetic nature of the bosonic field.¹⁷ The second term is proportional to $\Sigma 1/\sqrt{n}$ and also diverges but only as power $1/2$ in the ultraviolet and renormalizes a_h . To see this we calculate the sum

$$
\langle \varepsilon_A^n(k) + \varepsilon_O^n(k) \rangle_k = -2 + \frac{4}{\beta} \langle \langle |\varphi|^2 \varphi_k^{*n} \varphi_k^n \rangle_k \rangle_k = -2 + \frac{4}{\beta}.
$$
\n(43)

The last equality follows from the curious property of $\varphi_k^{*n}(x) \varphi_k^{n}(x)$ that it depends only on $x_i b - \varepsilon_{ij} k_j$. We see that apart from the renormalizations there is a finite correction:

$$
\frac{\mathcal{F}_{\text{fluc}}^{(1)}}{T} = 1.459 \left(-1 + \frac{2}{\beta} \right) \sigma b^{1/2} a_h \,. \tag{44}
$$

The following one is of the order $a_h²$ and will not be calculated here.

V. RESULTS FOR MAGNETIZATION AND SPECIFIC HEAT: RANGE OF APPLICABILITY OF THE LOOP EXPANSION AND GL APPROACH

Here we discuss the nature and range of applicability of the expansions we used for fluctuating superconductors (for which Gi is not negligibly small). There are two small parameters used. The first one is a_h/b which controls the expansion of the mean-field solution and, therefore, the HLL corrections were already discussed in Sec. III. The second small parameter controls the fluctuations. We assumed the mean field is the leading order and then expanded the statistical sum around it. Summarizing all the corrections the free energy density is

$$
\frac{\mathcal{F}}{T} = \omega^{-1} a_h^2 \bigg[c_2^{(-1)} + c_3^{(-1)} \frac{a_h}{b} + c_4^{(-1)} \bigg(\frac{a_h}{b} \bigg)^2 \bigg] \qquad (45)
$$

$$
+ \sigma b a_h^{1/2} \bigg[c_0^{(0)} \bigg(\frac{a_h}{b} \bigg)^{-1/2} + c_{1/2}^{(0)} + c_1^{(0)} \bigg(\frac{a_h}{b} \bigg)^{1/2}
$$

$$
+ c_{3/2}^{(0)} \frac{a_h}{b} \bigg] + \omega \sigma^2 b^2 a_h^{-1} \big[c_{-1}^{(1)} \big],
$$

where the coefficients (upper index is the power of ω and the lower index is the power of a_h) are

$$
c_2^{(-1)} = -0.434, \quad c_3^{(-1)} = -0.0078, \quad c_0^{(0)} = 0.526,
$$
\n(46)

$$
c_{1/2}^{(0)} = 316
$$
, $c_1^{(0)} = 1.06$, $c_{3/2}^{(0)} = -0.445$, $c_{-1}^{(1)} = 0.118$,

and ω is defined in Eq. (3). The last term is the two-loop contribution calculated in I. One clearly see that $\omega b a_h^{-3/2}$ always appears together with an important "loop factor" σ $= 1/2^{3/2} \pi \approx 0.11$. The expansion parameter therefore is

$$
\sigma \omega b a_h^{-3/2} = \pi \sqrt{2Gi} \frac{tb}{(1-t-b)^{3/2}} = \frac{1}{\sqrt{2\pi} |a_T|^{3/2}}.
$$

In the last equation a_T is the often used dimensionless LLL temperature introduced by Thouless.² For $Gi = 0.01$ the condition $\sigma \omega a_h^{-3/2}$ is represented by the area above the dotted line in Fig. 1.

Correspondingly the scaled magnetization is *m* $=-\frac{\partial \mathcal{F}}{\partial b}$:

$$
\frac{m}{T} = \omega^{-1} \left(c_2^{(-1)} a_h + \frac{3}{2} c_3^{(-1)} b^{-1} a_h^2 + 2 c_4^{(-1)} b^{-2} a_h^3 \right) + \sigma \left(c_3^{(-1)} \omega^{-1} b^{-2} a_h^3 - \frac{3}{2} c_0^{(0)} b^{1/2} - c_{1/2}^{(0)} a_h^{1/2} + \frac{1}{4} c_{1/2}^{(0)} b a_h^{-1/2} \right)
$$

$$
- \frac{1}{2} c_1^{(0)} b^{-1/2} a_h + \frac{1}{2} c_1^{(0)} b^{1/2} + \frac{3}{4} c_{3/2}^{(0)} a_h^{1/2} \right) - \omega \sigma^2 \left(2 b a_h^{-1} + \frac{1}{2} b^2 a_h^{-2} \right) \left[c_{-1}^{(1)} \right],\tag{47}
$$

while the scaled specific heat is $c = -t(\partial^2/\partial t^2)\mathcal{F}$:

$$
\frac{c}{t} = tT_c\omega^{-1} \left(-\frac{1}{2}c_2^{(-1)}\omega^{-1} - 3c_3^{(-1)}b^{-1}a_h - 9c_4^{(-1)}b^{-2}a_h^2 \right) + \sigma T_c \left(\frac{1}{2}c_{1/2}^{(0)}ba_h^{-1/2} + \frac{1}{16}c_{1/2}^{(0)}bta_h^{-3/2} + c_1^{(0)}b^{1/2} + \frac{3}{2}c_{3/2}^{(0)}a_h^{1/2} - \frac{3}{16}c_{3/2}^{(0)}ta_h^{-1/2} \right) + T_c\omega\sigma^2b^2 \left(a_h^{-2} - \frac{t}{2}a_h^{-3} \right) [c_{-1}^{(1)}].
$$
\n(48)

Now we address the question whether the GL energy itself can be reliably used in the region of applicability stated above. The GL free energy is an effective energy obtained after integrating out microscopic degrees of freedom φ_{micro} (for example, quantum electron fields in the BCS or Hubbard model). Formally one writes

$$
\exp\{-\beta F_{\text{GL}}[\psi]\} = \int_{\varphi_{\text{micro}}} \delta(\psi - \psi(\varphi_{\text{micro}})) \exp\{-\beta F[\varphi_{\text{micro}}]\},\tag{49}
$$

where the functional $F[\varphi_{\text{micro}}]$ describes a microscopic theory (one has to make also the quantum-mechanical average not shown explicitly). The order-parameter field is a function of the microscopic field (bilinear in electron field in BCS). Without detailed knowledge of the microscopic theory the functional $F_{\text{GL}}[\psi]$ could be quite general, however near T_c for $H=0$ or more generally near $H_{c2}(T)$ the order parameter is small and one can expand on it. Gorkov derived the coefficients of the GL theory from BCS.¹³ While some such derivations of the GL theory exist for high- T_c materials,¹⁸ also in the magnetic field, 19 here we show the consistency of the approach within the area of applicability of the approximation we use. Of course, in particular microscopic theories the range of applicability might be larger. Generally the requirements are the following. Terms $|\psi|^6, |\psi|^8, \ldots$ should be small compared to $|\psi|^4$ in the GL free energy Eq. (1). In addition gradients should be small so that higher (covariant) derivatives can be neglected compared to $|D\psi|^2$.

Our perturbative solution $\psi^{\alpha} \sqrt{a_h}$, therefore, $|\psi|^6 \propto a_h^3$ while $|\psi|^6 \propto a_h^2$. Therefore, in the leading order $|\psi|^6$ can be neglected. In higher orders, those higher terms do contribute. In the next leading term $|\psi|^6$ should be phenomenologically included, while $|\psi|^8$ not and so forth. As far as higher derivatives are concerned we have shown that even for HLL $|D\psi|^2 \propto ba_h$ and thus higher derivative terms appear only at quite high order. Therefore, we can take the GL free energy, Eq. (1) , as the free energy of the system to leading order. Thus in the LLL regime defined here in the paper, the GL theory shall describe the physics correctly. Higher-order corrections require more free parameters.

VI. CONCLUSION

In this paper we showed why the LLL results are often valid far beyond the naive limit of applicability of the approximation for both the mean-field and the fluctuation parts. Our results are valid strictly speaking between the longdashed line representing $H = H_{c2}(T)/13$ and one of the dashed curves indicating the range of validity of the loop expansion for the fluctuation contribution (depends on value of the Ginzburg number *Gi*). For nonfluctuating strongly type-II superconductors our results can be directly checked by experiments done at low temperature or numerical solution (or even the "London limit approximation") and are in clear agreement. For small, but not very small Ginzburg parameter *Gi* one can compare with existing Monte Carlo $~(\text{MC})$ simulations^{7,20} or experiments. Of course, one can use the existing high-temperature expansion² to interpolate to the present expansion range. Results for LLL were presented in I and the HLL do not alter them significantly. The agreement with the MC simulations is very good although obviously the melting transition is not seen. As argued in I it is not expected to exist within the present model. The HLL do not change this conclusion. That the ''supersoft'' *A* mode has a propagator $1/[k_z^2 + \text{const}(k_x^2 + k_y^2)^2]$ beyond the LLL approximation lays to rest a suspicion that this is a fluke due to LLL.¹⁵ This indicates that this unusual "softness" is due to some underlying symmetry which has yet to be explicitly identified.

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APPENDIX A: THIRD-ORDER CORRECTION TO THE MEAN-FIELD SOLUTION AND FREE ENERGY

In this appendix we provide some details of the third order correction in the *ah* calculation of the mean-field solution of the GL equations.

To calculate g_2^n , one takes the inner product of φ^n on the two sides of Eq. (14) and obtains Eq. (17) . To calculate g_2 , we need to consider the GL equation to order $a_h^{7/2}$:

$$
\mathcal{H}\Phi_3 = \Phi_2 - [(\Phi_0)^2 \Phi_2^* + (\Phi_1)^2 \Phi_0^* + 2 |\Phi_0|^2 \Phi_2
$$

+2|\Phi_1|^2 \Phi_0^*]. (A1)

The scalar product with φ gives Eq. (18).

Now we compute the a_h^4 order correction to free energy. Substituting Φ_2 from Eqs. (17) and (18) we find

$$
\frac{1}{2}a_h^3(\langle \Phi_2 | \mathcal{H} | \Phi_1 \rangle + \langle \Phi_1 | \mathcal{H} | \Phi_2 \rangle - \langle \Phi_2 | \Phi_0 \rangle - \langle \Phi_1 | \Phi_2 \rangle
$$

$$
-\langle \Phi_1 | \Phi_1 \rangle) = -\frac{g_2}{\beta^{1/2}}a_h^3 + a_h^3 \sum_{n=0} \left[n b g_1^n g_2^n - \frac{1}{2} (g_1^n)^2 \right].
$$
(A2)

Dominant contributions come from $\langle 6,6|0,0\rangle = \langle 0,0|6,6\rangle$ $= 0.80260, (6,0|6,0) = 0.80283$ and those coefficients are real.

APPENDIX B: SECOND-ORDER CORRECTION TO THE FLUCTUATIONS SPECTRUM

In this appendix we list matrix elements of the correction H_1 given by Eq. (27) between various states used in the calculation of the second-order correction to energies of excitations:

$$
\langle O_{k}|\hat{H}_{1}|O_{k}^{n}\rangle = \frac{1}{\beta} \langle |\varphi|^{2} (\varphi_{-\vec{k}}^{*}\varphi_{-\vec{k}}^{n} + \varphi_{\vec{k}}\varphi_{\vec{k}}^{*n}) \rangle
$$

+
$$
\frac{1}{2\beta} \langle \varphi^{*2} \varphi_{\vec{k}}\varphi_{-\vec{k}}^{n} + \varphi^{2} \varphi_{-\vec{k}}^{*}\varphi_{\vec{k}}^{*n} \rangle
$$

=
$$
\frac{1}{\beta} \bigg[\beta_{-\vec{k}}^{n} + \beta_{\vec{k}}^{*n} + \frac{1}{2} (\gamma_{-\vec{k}}^{n} + \gamma_{\vec{k}}^{*n}) \bigg], \quad \text{(B1)}
$$

$$
\langle A_{k}|\hat{H}_{1}|O_{k}^{n}\rangle = \frac{i}{\beta} \langle |\varphi|^{2} (\varphi_{\vec{k}}\varphi_{\vec{k}}^{*n} - \varphi_{-\vec{k}}^{n}\varphi_{-\vec{k}}^{*}) \rangle + \frac{i}{2\beta}
$$

$$
\times \langle \varphi^{*2} \varphi_{\vec{k}}\varphi_{-\vec{k}}^{n} - \varphi^{2} \varphi_{-\vec{k}}^{*}\varphi_{\vec{k}}^{*n} \rangle
$$

=
$$
\frac{i}{\beta} \bigg[-\beta_{-\vec{k}}^{n} + \beta_{\vec{k}}^{*n} + \frac{1}{2} (\gamma_{-\vec{k}}^{n} - \gamma_{\vec{k}}^{*n}) \bigg],
$$

 $|\langle O_k |\hat{H}_1 | O_k^n \rangle|^2 + |\langle O_k |\hat{H}_1 | A_k^n \rangle|^2$ $=\frac{2}{\beta^2}\left[\left|F_k^n(2)\right|^2+\left|F_{-k}^n(2)\right|\right]$ $(B4)$

$$
\langle A_k|\hat{H}_1|A_k^n\rangle\langle A_k^n|\hat{H}_1|O_k\rangle + \langle A_k|\hat{H}_1|O_k^n\rangle\langle O_k^n|\hat{H}_1|O_k\rangle + \text{c.c.}
$$

$$
= \frac{2}{\beta^2} [F_k^{*n}(1)F_k^n(2) - F_{-k}^n(1)F_{-k}^{*n}(2)] + \text{c.c.},
$$

where

$$
F_k^n(1) = \beta_k^n - \frac{1}{2} \gamma_k^n, \tag{B5}
$$

$$
F_k^n(2) = \beta_k^n + \frac{1}{2} \gamma_k^n.
$$

Finally, we can show that

$$
E_{\text{offdiag}} = -\frac{1}{b} \sum_{n} \frac{1}{n} \left\{ \frac{1}{\beta^2} \left[|F_{k}^{n}(1)|^2 + |F_{-k}^{n}(1)|^2 + |F_{k}^{n}(2)|^2 \right. \right. \\ \left. + |F_{-k}^{n}(2)|^2 \right] + \frac{\cos \theta_k}{\beta^2} \left[|F_{k}^{n}(1)|^2 + |F_{-k}^{n}(1)|^2 \right. \\ \left. - |F_{k}^{n}(2)|^2 - |F_{-k}^{n}(2)|^2 \right] \\ \left. + \frac{\sin \theta_k}{\beta^2} 2 \operatorname{Im} [F_{-k}^{n}(1) F_{-k}^{*n}(2) - F_{k}^{*n}(1) F_{k}^{n}(2)] \right\}. \tag{B6}
$$

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(B2)
\n
$$
\langle O_k | \hat{H}_1 | A_k^n \rangle = \frac{i}{\beta} \left[\beta_{-k}^n - \beta_k^{*n} + \frac{1}{2} (\gamma_{-k}^n - \gamma_k^{*n}) \right],
$$
\n
$$
\langle A_k^n | \hat{H}_1 | O_k \rangle = \frac{i}{\beta} \left[\beta_k^n - \beta_{-k}^{*n} + \frac{1}{2} (-\gamma_{-k}^{*n} + \gamma_k^n) \right],
$$
\n(B3)
\n
$$
\langle A_k | \hat{H}_1 | O_k^n \rangle = \frac{i}{\beta} \left[\beta_k^{*n} - \beta_{-k}^n + \frac{1}{2} (-\gamma_{-k}^n + \gamma_k^{*n}) \right],
$$
\n
$$
\langle O_k^n | \hat{H}_1 | O_k \rangle = \frac{1}{\beta} \left[\beta_{-k}^{*n} + \beta_k^n + \frac{1}{2} (\gamma_{-k}^{*n} + \gamma_k^n) \right],
$$

etc. From those formulas, we can show

 $|\langle A_k|\hat{H}_1|A_k^n\rangle|^2 + |\langle A_k|\hat{H}_1|O_k^n\rangle|^2 = \frac{2}{\beta^2} [|F_k^n(1)|^2 + |F_{-k}^n(1)|^2],$

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