Solid-State Calculation of Crystalline Color Superconductivity

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It is generally believed that the inhomogeneous Larkin-Ovchinnikov-Fulde-Ferrell (LOFF) phase appears in a color superconductor when the pairing between different quark flavors is under the circumstances of mismatched Fermi surfaces. However, the real crystal structure of the LOFF phase is still unclear because an exact treatment of 3D crystal structures is rather difficult. In this work we calculate the ground-state energy of the body-centered cubic (BCC) structure for two-flavor pairing by diagonalizing the Hamiltonian matrix in the Bloch space, in analogy to the ab initio calculations in solid-state physics. We develop a computational scheme to overcome the difficulties in diagonalizing huge matrices. Our results show that the BCC structure is energetically more favorable than the 1D modulation in a narrow window around the conventional LOFF-normal phase transition point, which indicates the significance of the higher-order terms in the Ginzburg-Landau approach.

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The ground state of exotic fermion Cooper pairing with mismatched Fermi surfaces is a longstanding problem in the theory of superconductivity [1]. In electronic superconductors, the mismatched Fermi surfaces are normally induced by the Zeeman energy splitting $2\delta\mu$ in a magnetic field. For s-wave pairing at weak coupling, it is known that, at a critical field $\delta\mu_1 = 0.707\Delta_0$ where $\Delta_0$ is the pairing gap at vanishing mismatch, a first-order phase transition from the gapped BCS state to the normal state occurs [2]. Further theoretical studies showed that the inhomogeneous Larkin-Ovchinnikov-Fulde-Ferrell (LOFF) state can survive in a narrow window $\delta\mu_1 < \delta\mu < \delta\mu_2$, where the upper critical field $\delta\mu_2 = 0.754\Delta_0$ [3, 4]. However, since the thermodynamic critical field is much lower than $\delta\mu_1$ due to strong orbit effect, it is rather hard to observe the LOFF state in ordinary superconductors [5]. In recent years, experimental evidences for the LOFF state in some superconducting materials have been reported [5-8].

On the other hand, exotic pairing phases have promoted new interest in the studies of dense quark matter under the circumstances of compact stars [6, 9] and ultracold atomic Fermi gases with population imbalance [20, 21]. Color superconductivity in dense quark matter appears due to the attractive interactions in certain diquark channels [22, 23]. Because of the constraints from Beta equilibrium and electric charge neutrality, different quark flavors ($u$, $d$, and $s$) acquire mismatched Fermi surfaces. Quark color superconductors under compact-star constraints as well as atomic Fermi gases with population imbalance therefore provide rather clean systems to realize the long-sought exotic LOFF phase.

Around the tricritical point in the temperature-mismatch phase diagram, the LOFF phase can be studied rigorously by using the Ginzburg-Landau (GL) analysis since both the gap parameter and the pair momentum are vanishingly small [11]. It was found that the solution with two antipodal wave vectors is the preferred one [23, 24]. However, the real ground state of the LOFF phase is still debated due to the limited theoretical approaches at zero temperature. So far rigorous studies of the LOFF phase at zero temperature are restricted to its 1D structures including the Fulde-Ferrell (FF) state with a plane-wave form $\Delta(z) = e^{i2qz}$ and the Larkin-Ovchinnikov (LO) state with an antipodal-wave form $\Delta(z) = 2\alpha \cos(2qz)$. A recent self-consistent treatment of the 1D modulation [30] showed that a solitonic lattice is formed near the lower critical field, and the phase transition to the BCS state is continuous. Near the upper critical field the gap function becomes sinusoidal, and the transition to the normal state is of first order.

In addition to these 1D structures, there exist a large number of 3D crystal structures. The general form of a crystal structure of the order parameter can be expressed as

$$\Delta(r) = \sum_{k=1}^{P} e^{i2q_k r}.$$  (1)

A specific crystal structure corresponds to a multi-wave configuration determined by the $P$ unit vectors $q_k (k = 1, 2, ..., P)$. In general, we expect two competing mechanisms: Increasing the number of waves tends to lower the energy, but it may also causes higher repulsive interaction energy between different wave directions. In a pioneer work, Bowers and Rajagopal investigated 23 different crystal structures by using the GL approach [10], where the grand potential measured with respect to the normal state was expanded up to the order $O(\Delta^6)$,

$$\frac{\delta\Omega(\Delta)}{N_F} = P\alpha\Delta^2 + \frac{1}{2}\beta\Delta^4 + \frac{1}{3}\gamma\Delta^6 + O(\Delta^8)$$  (2)

with $N_F$ being the density of state at the Fermi surface and the pair momentum fixed at the optimal value $q = 1.1997\delta\mu$. Among the structures with $y > 0$, the favored one seems to be the body-centered cubic (BCC) with $P = 6$ [31]. Further, it was conjectured that the face-centered cubic (FCC) with $P = 8$ [32] is the preferred structure since its $y$ is negative and the largest [10]. For BCC structure, the GL analysis up to the order $O(\Delta^6)$ predicts a strong first-order phase transition at $\delta\mu_c \approx 3.6\Delta_0$ with the gap parameter $\Delta \approx 0.8\Delta_0$ [10]. However, by using the quasiclassical equation approach, Combescot and Mora [33, 34] predicted that the BCC-normal transition is of rather weak first order: The upper critical field $\delta\mu_c$ is only
about 4% higher than $\delta \mu_2$ with $\Delta \approx 0.1 \Delta_0$ at $\delta \mu = \delta \mu_\ast$. If this result is reliable, it indicates that the higher-order expansions in the GL analysis is important for quantitative predictions. To understand this intuitively, let us simply add the eighth-order term $\frac{\eta^2}{\Lambda^8}$ to the GL potential \[^4\]. For $\eta \rightarrow +\infty$, the phase transition becomes of weak first order and $\delta \mu_\ast \rightarrow \delta \mu_2$ \[^5\]. Therefore, to give more precise predictions we need to study the higher-order expansions and the convergence property of the GL series, or use a different way to evaluate the grand potential without assuming $\Delta$ is small.

In this work, we present for the first time calculation of the grand potential of the BCC structure in analogy to the \textit{ab initio} calculation of the electronic band structure in solid-state physics. Here, the crystalline structure of the order parameter plays a similar role of the periodic potentials in solids.

To be specific, we consider a general effective Lagrangian for two-flavor quark pairing at high density. The Lagrangian density is given by $\mathcal{L} = \bar{\psi} \left[ i \gamma_\mu \partial^\mu - \mathbf{e} \cdot \mathbf{p} + \mu \right] \psi + \mathcal{L}_{\text{int}}$, where $\psi = (\psi_u, \psi_d)^T$ denotes the two-flavor quark field and $e(\mathbf{p})$ is the quark dispersion with $\mathbf{p} = -i\nabla$. The quark chemical potentials are specified by the diagonal matrix $\hat{\mu} = \text{diag}(\mu_u, \mu_d)$ in the flavor space, where $\mu_u = \mu + \delta \mu$ and $\mu_d = \mu - \delta \mu$. The interaction Lagrangian density which leads to Cooper pairing between different flavors can be expressed as \[^1\]

$$\mathcal{L}_{\text{int}} = g(\psi_1 \sigma_2 \psi_2)(\psi_2^T \sigma_2 \psi_1),$$  

(3)

where $g$ is the coupling constant and $\sigma_2$ is the second Pauli matrix in the flavor space.

Color superconductivity is characterized by nonzero expectation value of the diquark field $\varphi(t, \mathbf{r}) = -2ig\bar{\psi}^T \sigma_2 \psi$. For the purpose of studying inhomogeneous phases, we set the expectation value of $\varphi(t, \mathbf{r})$ to be static but inhomogeneous, i.e., $\langle \varphi(t, \mathbf{r}) \rangle = \Delta(\mathbf{r})$. With the Nambu-Gor’kov spinor $\Psi = (\psi, \psi^\dagger)^T$, the mean-field Lagrangian reads

$$\mathcal{L}_{\text{MF}} = \frac{1}{2} \Psi^T \left( \begin{array}{cc} -\mathbf{i} \partial_t - e(\mathbf{p}) + \mu & -i \sigma_2 \Delta(\mathbf{r}) \\ i \sigma_2 \Delta^*(\mathbf{r}) & -\mathbf{i} \partial_t + e(\mathbf{p}) - \mu \end{array} \right) \Psi - \frac{|\Delta(\mathbf{r})|^2}{4g},$$

(4)

The order parameters of the BCC and FCC structures can be expressed as

$$\Delta(\mathbf{r}) = 2\Delta \cos(2q_1x) \cos(2q_2y) \cos(2q_3z),$$

(5)

and

$$\Delta(\mathbf{r}) = 8\Delta \cos \left( \frac{2q_1}{\sqrt{3}} \right) \cos \left( \frac{2q_2}{\sqrt{3}} \right) \cos \left( \frac{2q_3}{\sqrt{3}} \right),$$

(6)

respectively. Therefore, we consider a 3D periodic structure where the unit cell is spanned by three linearly independent vectors $\mathbf{a}_1 = a \mathbf{e}_x$, $\mathbf{a}_2 = a \mathbf{e}_y$, and $\mathbf{a}_3 = a \mathbf{e}_z$ with $a = \pi/q$ for BCC and $a = \sqrt{3}\pi/q$ for FCC. The order parameter is periodic in space, i.e., $\Delta(\mathbf{r}) = \Delta(\mathbf{r} + \mathbf{a})$. It can be decomposed into a discrete set of Fourier components,

$$\Delta(\mathbf{r}) = \sum_\mathbf{G} \Delta_\mathbf{G} e^{i\mathbf{G} \cdot \mathbf{r}},$$

(7)

where the reciprocal lattice vector $\mathbf{G}$ reads

$$\mathbf{G} = \frac{2\pi}{a} (l \mathbf{e}_x + m \mathbf{e}_y + n \mathbf{e}_z), \quad l, m, n \in \mathbb{Z}.$$  

(8)

The Fourier component $\Delta_\mathbf{G}$ can be evaluated as

$$\Delta_\mathbf{G} = \Delta \left[ (\delta_{l,1} + \delta_{l,-1}) \delta_{m,0} \delta_{n,0} + \delta_{l,0} (\delta_{m,1} + \delta_{m,-1}) \delta_{n,0} \\ + \delta_{l,0} \delta_{m,0} (\delta_{n,1} + \delta_{n,-1}) \right]$$

(9)

and

$$\Delta_\mathbf{G} = \Delta \left( \delta_{l,1} + \delta_{l,-1} \right) (\delta_{m,1} + \delta_{m,-1}) (\delta_{n,1} + \delta_{n,-1})$$

(10)

for BCC and FCC structures, respectively.

Then we consider a finite system in a cubic box defined as $x, y, z \in [-L/2, L/2]$ with the length $L = Na$. The thermodynamic limit is reached by setting $N \rightarrow \infty$. Using the periodic boundary condition, we have the Fourier transformation $\Psi(\mathbf{r}, \mathbf{p}) = V^{-1/2} \sum_\mathbf{p} \Psi_\mathbf{p} e^{i(\mathbf{r} - \mathbf{p}) \cdot \mathbf{p} / Na}$, where $V$ is the volume of the system. The partition function $\mathcal{Z} = \int [d\Psi][d\Psi^\dagger] e^{-S}$ with the Euclidean action

$$S = -\int_0^{1/T} dt \int d^3v \mathcal{L}. \quad \text{Using the Fourier expansions for } \Psi \text{ and } \Delta, \text{ we obtain the mean-field action}$$

$$S_{\text{MF}} = \frac{V}{T} \sum_\mathbf{G} \frac{|\Delta_\mathbf{G}|^2}{4g} - \frac{1}{2T} \sum_\mathbf{p} \sum_\mathbf{p} \Psi^\dagger_\mathbf{p} \left( \omega_\mathbf{p} \delta_{\mathbf{p}, \mathbf{p}} - \mathcal{H}_{\mathbf{p}, \mathbf{p}} \right) \Psi_\mathbf{p},$$

(11)

where the effective Hamiltonian matrix $\mathcal{H}_{\mathbf{p}, \mathbf{p}}$ reads

$$\mathcal{H}_{\mathbf{p}, \mathbf{p}} = \left( \begin{array}{cc} (|\mathbf{p}| - \mu) \delta_{\mathbf{p}, \mathbf{p}} & i \sigma_2 \sum_\mathbf{G} \Delta_\mathbf{G} \delta_{\mathbf{G}, \mathbf{p} - \mathbf{p}} \\ -i \sigma_2 \sum_\mathbf{G} \Delta_\mathbf{G} \delta_{\mathbf{G}, \mathbf{p} - \mathbf{p}} & -(|\mathbf{p}| - \mu) \delta_{\mathbf{p}, \mathbf{p}} \end{array} \right).$$

(12)

The effective Hamiltonian $\mathcal{H}_{\mathbf{p}, \mathbf{p}}$ is a huge matrix in Nambu–Gor’kov, color, flavor, spin, and (discrete) momentum spaces. It is Hermitian and can in principle be diagonalized. Assuming the eigenvalues of $\mathcal{H}_{\mathbf{p}, \mathbf{p}}$ is denoted by $E_\lambda$, we can formally express the grand potential as

$$\Omega = \frac{1}{4g} \sum_\mathbf{G} |\Delta_\mathbf{G}|^2 - \frac{1}{2V} \sum_\lambda \mathcal{W}(E_\lambda),$$

(13)

where the function $\mathcal{W}(E) = \frac{E}{T} + T \ln(1 + e^{-E/T})$. The summation over $\mathbf{G}$ can be worked out as $\sum_\mathbf{G} |\Delta_\mathbf{G}|^2 = P \Delta^2$.

In practice, diagonalization of the matrix $\mathcal{H}_{\mathbf{p}, \mathbf{p}}$ is infeasible. However, $\mathcal{H}$ can be brought into a block-diagonal form with $N^3$ independent blocks in the momentum space according to the famous Bloch theorem. To understand this, we consider the eigenvalue equation in coordinate space or the so-called Bogoliubov-de Gennes (BdG) equation

$$\left( \begin{array}{cc} e(-\nabla) - \mu & i \sigma_2 \Delta(\mathbf{r}) \\ -i \sigma_2 \Delta^*(\mathbf{r}) & e(-\nabla) + \mu \end{array} \right) \phi_\lambda(\mathbf{r}) = E_\lambda \phi_\lambda(\mathbf{r}).$$

(14)

According to the Bloch theorem, the solution of the eigenfunction $\phi_\lambda(\mathbf{r})$ can be expressed as $\phi_\lambda(\mathbf{r}) = e^{ik \cdot \mathbf{G}} \phi_\lambda(\mathbf{r})$, where
\[ k \] is the momentum in the Brillouin zone (BZ) and the function \( \phi_{k}(r) \) has the same periodicity as the order parameter. We therefore have the similar Fourier expansion \( \phi_{k}(r) = \sum_{G} \phi_{G}(k)e^{iG \cdot r} \). Substituting this expansion into the BdG equation, for a given \( k \) we obtain a matrix equation

\[
\sum_{G} \mathcal{H}_{G,G'}(k)\phi_{G'}(k) = E_{G}(k)\phi_{G}(k),
\]

where the matrix \( \mathcal{H}_{G,G'}(k) \) is given by

\[
\begin{pmatrix}
(k + G) - \mu & i\sigma_{2} \Delta_{G,G'} \\
-i\sigma_{2} \Delta_{G,-G} & -(k + G) - \mu
\end{pmatrix}.
\]

This shows that, for a given \( k \)-point in the BZ, we can solve the eigenvalue \( E_{i}(k) \) by diagonalizing the matrix \( \mathcal{H} \). Without loss of generality, the BZ can be chosen as \( k_{x}, k_{y}, k_{z} \in [-\pi/a, \pi/a] \). For a quantized volume \( V \) containing \( N^{3} \) unit cells, we have \( N^{3} \) allowed momenta \( k \) in the BZ. Accordingly, the grand potential is now given by

\[
\Omega = \frac{P\Delta^{2}}{4g} - \frac{1}{2V} \sum_{k \in \text{BZ}} \sum_{\Delta} \mathcal{W}[E_{i}(k)].
\]

In the thermodynamic limit \( N \to \infty \), the summation \( \sum_{k \in \text{BZ}} \) is replaced by an integral over the BZ.

The Hamiltonian matrix \( \mathcal{H}_{G,G'}(k) \) can be further simplified to lower the matrix size. After a proper rearrangement of the eigenstate \( \phi_{G} \), we find that \( \mathcal{H} \) can be decomposed into two blocks. We have \( \mathcal{H} = \mathcal{H}_{\Delta,\delta\mu} \oplus \mathcal{H}_{-\Delta,\delta\mu} \). The blocks can be expressed as \( \mathcal{H}_{\Delta,\delta\mu} = \mathbf{H} - \delta\mu \mathbf{I} \) where the matrix \( \mathbf{H} \) is given by

\[
\begin{pmatrix}
(k + G) - \mu & \Delta_{G,G'} \\
-\Delta_{G,-G} & -(k + G) - \mu
\end{pmatrix}.
\]

The eigenvalues of \( \mathcal{H}_{\Delta,\delta\mu} \) do not depend on the sign of \( \Delta \). Moreover, replacing the \( \delta\mu \) by \( -\delta\mu \) amounts to a replacement of the eigenvalue spectrum \( \{E_{i}(k)\} \) by \( \{-E_{i}(k)\} \). Therefore, the two blocks contribute equally to the grand potential and we only need to determine the eigenvalues of \( \mathcal{H}_{\Delta,\delta\mu} \). The Hamiltonian matrix \( \mathcal{H}_{\Delta,\delta\mu} \) is replaced by an integral over the BZ.

In the following we shall focus on the zero-temperature case. The grand potential \( \Omega \) is divergent and hence a proper regularization scheme is needed. Since we need to deal with the Bloch momentum \( k + G \), the usual three-momentum cutoff scheme is not appropriate for numerical calculations. Moreover, we are interested in the grand potential \( \delta\Omega \) measured with respect to the normal state. Therefore, we employ a Pauli-Villars-like regularization scheme, in which \( \delta\Omega \) is well-defined. The “renormalized” grand potential is given by \( \delta\Omega(\Delta, q) = \Omega(\Delta, q) - \Omega(0, q) \), where

\[
\Omega(\Delta, q) = \frac{P\Delta^{2}}{4g} - \frac{1}{2V} \sum_{k \in \text{BZ}} \sum_{\Delta} \sum_{j=0}^{2} \sum_{\mu} \langle \mathcal{E}_{j}(k) + j\Delta \rangle
\]

with \( c_{0} = c_{2} = 1 \) and \( c_{1} = -2 \). Here \( \{\mathcal{E}_{j}(k)\} \) denotes the eigenvalue spectrum of \( \mathcal{H}_{\Delta,\delta\mu} \). The coupling constant \( g \) can be fixed by the BCS gap \( \Delta_{0} \) at \( \delta\mu = 0 \). We expect that at weak coupling the physical results depend on the cutoff \( \Lambda \) only through the BCS gap \( \Delta_{0} \). In Fig. 1 we show the stability window for the FF state as a function of \( \Delta_{0} \). The inset shows the window size \( (\delta\mu_{2} - \delta\mu_{1})/\Delta_{0} \).

![FIG. 1: (Color online) The stability window for the FF state as a function of \( \Delta_{0} \) at \( \mu = 400 \text{ MeV} \). The thin lines denote results in the weak-coupling limit. The thick solid and dashed lines correspond to \( \Lambda = 400 \text{ MeV} \) and \( \Lambda = 800 \text{ MeV} \), respectively. The insert shows the window size \( (\delta\mu_{2} - \delta\mu_{1})/\Delta_{0} \).](image)
from the LO state. The calculation of the LO state is much easier than 3D structures because the matrix size becomes $2D + 1$ [35]. For $\Delta_0 \sim 100$ MeV we need $k_{\text{max}} \simeq 5\text{GeV}$ [39]. Since we are interested in the region $\delta\mu/\Delta_0 \in [0.7, 0.8]$ and the optimal pair momentum is $q \sim \delta\mu$, we estimate $D \sim 35$ for BCC and $D \sim 60$ for FCC. These huge matrix sizes are beyond the capability of our current computing facility. On the other hand, even though a supercomputer may be able to diagonalize these huge matrices, the computing time and cost are still enormous, which makes the calculation infeasible.

Since we are interested in the grand potential $\delta\Omega$ rather than the band structure (the eigenvalues), we can neglect a small amount of the off-diagonal couplings $A$ in the matrix $H_\perp$. By doing so, the huge matrix $H_\perp$ can be decomposed into a number of blocks with size $(2d + 1)^3$ [35]. For symmetry reason, we set the centers of these blocks at the reciprocal lattice vectors $G = (2d + 1)\pi/(n_xa + n_yb + n_zc)$ with $n_x, n_y, n_z \in \mathbb{Z}$. With increasing $d$, the grand potential converges to the result from exact diagonalization. Good convergence is normally reached at some value $d = d_0$ [35]. If the block size $(2d_0 + 1)^3$ is within our computing capability, the calculation becomes feasible. Fortunately, we find that this computational scheme works for the BCC structure. At present, we are not able to perform a calculation for the FCC structure, since the value of $d_0$ needed for convergence is much larger. Note that the computing cost is still very large even though we have employed this effective computational scheme.

We have performed calculations of the BCC structure for $\Delta_0 = 60, 80, 100$ MeV [47] at $\mu = 400$ MeV [40]. For different values of $\Delta_0$, the results are almost the same in terms of the quantity $(\delta\mu - \delta\mu_2)/\Delta_0$. Therefore, we anticipate that our results can be appropriately extrapolated to the weak coupling limit $\Delta_0 \rightarrow 0$. In the following, we shall present the result for $\Delta_0 = 100$ MeV. For a given value of $\delta\mu/\Delta_0$, we calculate the potential curve $\delta\Omega(\Delta)$ at various values of $q$ and search for the optimal pair momentum and the minimum of the potential landscape. The potential curves at the optimal pair momenta for several values of $\delta\mu/\Delta_0$ are shown in Fig. 2 With increasing value of $\delta\mu/\Delta_0$, the potential minimum gets shallower. At a critical value $\delta\mu_1 - \delta\mu_2 \simeq 0.03\Delta_0$, the potential minimum approaches zero and a first-order phase transition to the normal state occurs. The comparison of the grand potentials of various phases are shown in Fig. 3 For the LO state, its phase transition to the normal state occur almost at the same point as the FF state, $\delta\mu_2 \simeq 0.8\Delta_0$. At $\delta\mu = \delta\mu_2$, the grand potential of the BCC structure is negative, which indicates that the BCC structure is energetically favored around the FF-normal transition point. Well below the FF-normal transition point, the BCC state has higher grand potential than the LO state and hence is not favored. Near the BCS-LO transition, the solitonic state becomes favored [30]. However, this does not change our qualitative conclusion.

Our result is qualitatively consistent with the GL analysis [10]. However, the quantitative difference is significant: The GL analysis predicts a strong first-order phase transition and a large upper critical field [10], while our result shows a weak first-order phase transition at which $\Delta \approx 0.1\Delta_0$. On the other hand, our result is quantitatively compatible with the quasiclassical equation approach [33,34], where it shows that the BCC structure is preferred in a narrow window around $\delta\mu = \delta\mu_2$ at zero temperature [41]. Therefore, the GL analysis up to the order $O(\Delta^3)$ may not be quantitatively sufficient. We notice that the LO state already shows the limitation of the GL analysis: While the GL analysis predicts a second-order phase transition, exact calculation shows a first-order phase transition in 3D [31]. In the future, it is necessary to study the higher-order expansions and the convergence property of the GL series, which would help to quantitatively improve the GL predictions.

In summary, we have performed for the first time an ab-initio-like calculation of the ground-state energy of a 3D struc-

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**FIG. 2:** (Color online) The potential curves $\delta\Omega(\Delta)$ of the BCC structure at the optimal pair momenta for various values of $\delta\mu/\Delta_0$. The red dots show the data obtained from our numerical calculation.

**FIG. 3:** (Color online) Comparison of the grand potentials of various phases: BCS (black solid), FF (blue dotted), LO (green dash-dotted), and BCC (red dashed). The horizontal axis has been “calibrated” by using the quantity $(\delta\mu - \delta\mu_2)/\Delta_0$. 

ture in crystalline color superconductivity. We proposed a computational scheme to overcome the difficulties in diagonalizing matrices of huge sizes. Our numerical results show that the BCC structure is preferred in a small window around the conventional FF-normal phase transition point, which indicates that the higher-order terms in the GL approach are rather important. In the future it would be possible to perform a calculation for the FCC structure with stronger computing facilities. This ab-initio-like approach can also be applied to study the crystalline structures of the three-flavor color-superconducting quark matter and the inhomogeneous chiral condensate.

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1. R. Casalbuoni and G. Nardulli, Rev. Mod. Phys. 76, 263 (2004).
2. B. S. Chandrasekhar, Appl. Phys. Lett. 1, 7 (1962); A. M. Clogston, Phys. Rev. Lett. 9, 266 (1962).
3. A. I. Larkin and Y. N. Ovchinnikov, Zh. Eksp. Teor. Fiz. 47, 1136 (1964).
4. P. Fulde and R. A. Ferrell, Phys. Rev. 135, A550 (1964).
5. K. Gloos, et. al., Phys. Rev. Lett. 70, 501 (1993); R. Modler, et. al., ibid 76, 1292 (1996); A. Bianchi, et. al., ibid 91, 187004 (2003).
6. J. L. O’Brien, et. al., Phys. Rev. B61, 1584 (2000).
7. L. Balicas, et. al., Phys. Rev. Lett. 87, 067002 (2001); M. A. Tanatar, et. al., Phys. Rev. B66, 134503 (2002).
8. S. Kasahara, et. al., Proc. Natl. Acad. Sci. 111, 16309 (2014).
9. M. Alford, J. Bowers, and K. Rajagopal, Phys. Rev. D63, 074016 (2001).
10. J. A. Bowers, K. Rajagopal, Phys. Rev. D66, 065002 (2002).
11. I. Shovkovy and M. Huang, Phys. Lett. B564, 205 (2003).
12. M. Alford, C. Kouvaris, and K. Rajagopal, Phys. Rev. Lett. 92, 222001 (2004).
13. R. Casalbuoni, M. Cininale, M. Mannarelli, G. Nardulli, M. Ruggieri, and R. Gatto, Phys. Rev. D70, 054004 (2004).
14. M. Huang and I. Shovkovy, Phys. Rev. D70, 051501(R) (2004).
15. R. Casalbuoni, R. Gatto, M. Mannarelli, G. Nardulli, and M. Ruggieri, Phys. Lett. B605, 362 (2005).
16. K. Fukushima, Phys. Rev. D72, 074002 (2005).
17. I. Giannakis and H.-C. Ren, Phys. Lett. B611, 137 (2005).
18. E. V. Gorbar, M. Hashimoto, and V. A. Miransky, Phys. Rev. Lett. 96, 022005 (2006).
19. R. Anglani, R. Casalbuoni, M. Cininale, R. Gatto, N. Ippolito, M. Mannarelli, and M. Ruggieri, Rev. Mod. Phys. 86, 509 (2014).
20. M. W. Zwierlein, et. al., Science 311, 492 (2006); G. B. Partridge, et. al., ibid 311, 503 (2006).
21. D. E. Sheehy and L. Radzihovsky, Phys. Rev. Lett. 96, 060401 (2006).
22. M. Alford, K. Rajagopal, and F. Wilczek, Phys. Lett. B422, 247 (1998).
23. R. Rapp, T. Schaefer, E. V. Shuryak, and M. Velkovsky, Phys. Rev. Lett. 81, 53 (1998).
24. M. Alford, K. Rajagopal, and F. Wilczek, Nucl. Phys. B537, 443 (1999).
25. D. T. Son, Phys. Rev. D59, 094019 (1999).
26. M. Alford, K. Rajagopal, T. Schaefer, and A. Schmitt, Rev. Mod. Phys. 80, 1455 (2008); D. H. Rischke, Prog. Part. Nucl. Phys. 52, 197 (2004); M. Buballia, Phys. Rep. 407, 205 (2005); I. A. Shovkovy, Found. Phys. 35, 1309 (2005).
27. A. I. Buzdin and H. Kachkachi, Phys. Lett. A225, 341 (1997).
28. R. Combescot and C. Mora, Eur. Phys. J. B28, 397 (2002).
29. L. Jiang and J. Ye, Phys. Rev. B76, 184104 (2007).
30. D. Nickel and M. Buballia, Phys. Rev. D79, 054009 (2009).
31. The six unit vectors of BCC structure are given by
\[ \hat{\mathbf{n}}_1 = (+1,0,0), \hat{\mathbf{n}}_2 = (-1,0,0), \hat{\mathbf{n}}_3 = (0,+1,0), \hat{\mathbf{n}}_4 = (0,-1,0), \hat{\mathbf{n}}_5 = (0,0,+1), \hat{\mathbf{n}}_6 = (0,0,-1). \]
32. The eight unit vectors of FCC structure are given by
\[ \hat{\mathbf{n}}_1 = (+k, +k, +k), \hat{\mathbf{n}}_2 = (-k, -k, -k), \hat{\mathbf{n}}_3 = (+k, -k, +k), \hat{\mathbf{n}}_4 = (-k, -k, +k), \hat{\mathbf{n}}_5 = (+k, +k, -k), \hat{\mathbf{n}}_6 = (-k, +k, -k), \hat{\mathbf{n}}_7 = (-k, -k, -k), \hat{\mathbf{n}}_8 = (+k, -k, -k), \]
where \( k = 1/\sqrt{3}. \)
33. R. Combescot and C. Mora, EPL 68, 79 (2004).
34. C. Mora and R. Combescot, Phys. Rev. B 71, 214504 (2005).
35. For details, see Supplemental Material.
36. The grand potential \( \Omega(\Delta, q) \) is still logarithmically divergent after applying the Pauli-Villars regularization. However, by subtracting \( \Omega(0, q) \) for the normal state, \( \delta\Omega(\Delta, q) \) is well defined.
37. For very small values of \( \Delta_0 \) (such as \( \Delta_0 = 20 \) MeV), the grand potential \( \delta\Omega \) becomes very small. We therefore need much higher accuracy in diagonalizing the matrices, which leads to much larger computing time and cost.
38. We compare the results obtained by using different numbers of \( k \)-points to check the convergence to the thermodynamic limit.
39. Note that decreasing the value of \( \Delta_0 \) does not help to reduce the matrix size. With decreasing \( \Delta_0 \) (even though \( k_{\text{max}} \) becomes smaller, the optimal pair momentum also gets smaller.
40. The parameter \( \Lambda \) for the Pauli-Villars regularization is chosen as \( \Lambda = 400 \) MeV. However, we checked that a different choice of \( \Lambda \) does not leads to a qualitative different result.
41. See Fig. 12 of Ref. [24] for details.
42. M. Mannarelli, K. Rajagopal, and R. Sharma, Phys. Rev. D73, 114012 (2006); K. Rajagopal and R. Sharma, Phys. Rev. D74, 094019 (2006).
43. M. Buballia and S. Carignano, arXiv:1406.1367.
Supplemental Material

Ginzburg-Landau Theory: Importance of Higher Order Expansions

In the zero-temperature Ginzburg-Landau (GL) theory of crystalline color superconductivity, the grand potential measured with respect to the normal state, \( \Omega = \Omega - \Omega_N \), is expanded as

\[
\frac{\delta \Omega(\Delta)}{N_F} = \rho \Delta^2 + \frac{1}{2} \xi \Delta^4 + \frac{1}{3} \gamma \Delta^6 + \frac{1}{4} \eta \Delta^8 + O(\Delta^{10}),
\]

(20)

where \( N_F \) is the density of state at the Fermi surface. The coefficient \( \rho \) is universal for all crystal structures. At weak coupling, it is given by

\[
\alpha = -1 + \frac{\delta \mu}{2q} \ln \frac{q + \delta \mu}{q - \delta \mu} - \frac{1}{2} \ln \left( \frac{\Delta_0^2}{4(q^2 - \delta \mu^2)} \right).
\]

(21)

Let us consider the vicinity of the conventional LOFF-normal transition point \( \delta \mu = \delta \mu_2 \), where we have

\[
\frac{\delta \mu_2}{\Delta_0} = 0.7544, \quad \frac{q}{\delta \mu_2} = 1.1997.
\]

(22)

At the pair momentum \( q = 1.1997 \delta \mu \), we have

\[
\alpha = \ln \frac{\delta \mu}{\Delta_0} - \ln \frac{\delta \mu_2}{\Delta_0} = \ln \frac{\delta \mu}{\delta \mu_2}.
\]

(23)

The GL potential becomes dimensionless if we employ the variables \( \delta \Omega = \delta \Omega/(N_0 \delta \mu^2) \), \( \bar{\Lambda} = \Lambda/\delta \mu \), \( \beta = \beta \delta \mu^2 \), \( \gamma = \gamma \delta \mu^4 \), and \( \bar{\eta} = \eta \delta \mu^6 \). We obtain

\[
\bar{\Omega} = \rho \bar{\Lambda}^2 + \frac{1}{2} \bar{\xi} \bar{\Lambda}^4 + \frac{1}{3} \bar{\gamma} \bar{\Lambda}^6 + \frac{1}{4} \bar{\eta} \bar{\Lambda}^8 + O(\bar{\Lambda}^{10}).
\]

(24)

The GL coefficients \( \beta \) and \( \gamma \) for a number of crystalline structures were first calculated by Bowers and Rajagopal [1]. The predictions for the nature of the phase transitions were normally based on the GL potential up to the sixth order (\( \Delta^6 \)). To our knowledge, the higher order GL coefficients have never been calculated. Here we do not intend to do this calculation. We shall show that the higher order GL expansions are important for the prediction of the phase transition point and the nature of the phase transition. To be specific, let us consider the BCC structure. Its GL coefficients \( \beta \) and \( \gamma \) have been evaluated as

\[
\beta = -31.466, \quad \gamma = 19.711.
\]

(25)

Since \( \beta < 0 \), the phase transition to the normal state should be of first order. If we employ the GL potential up to the sixth order, we predict a strong first-order phase transition at \( \delta \mu = \delta \mu_2 = 3.625 \Delta_0 \). However, here we show that the size of the coefficient \( \bar{\eta} \) is important for the study of the phase transition. In Fig. 4, we show the GL potential curves for two different values of \( \bar{\eta} \) at \( \delta \mu = \delta \mu_2 \). For vanishing \( \bar{\eta} \), the potential curve develops a deep minimum \( \delta \bar{\Omega}_{\min} \approx -13.4 \) at \( \Delta = 0.95 \Delta_0 \), which indicates a strong first-order phase transition at \( \delta \mu = \delta \mu_2 \Rightarrow \delta \mu_2 \). However, for a large value \( \bar{\eta} = 1000 \), we find a shallow minimum \( \delta \bar{\Omega}_{\min} \approx -0.21 \) located at \( \Delta \approx 0.31 \Delta_0 \). In Fig. 5, we show the GL potential curves at the first-order phase transition point \( \delta \mu = \delta \mu_2 \). For \( \bar{\eta} = 0 \) we find a strong first-order phase transition at \( \delta \mu = \delta \mu_2 = 3.625 \Delta_0 \), where the minima located at \( \Delta = 0 \) and \( \Delta = 0.83 \Delta_0 \) become degenerate. For \( \bar{\eta} = 1000 \), however, we observe a much weaker first-order phase transition at \( \delta \mu = \delta \mu_2 = 0.951 \Delta_0 \), where the minima located at \( \Delta = 0 \) and \( \Delta = 0.28 \Delta_0 \) are degenerate. These results clearly show that, for larger \( \bar{\eta} \), the first-order phase transition becomes weaker. For \( \bar{\eta} \to +\infty \), we expect that \( \delta \mu_2 \to 0.754 \Delta_0 \). On the other hand, if \( \bar{\eta} \) is small or even negative, then the next order \( \Delta^{10} \) would become important.

Matrix Structures of BCC and FCC Crystals

To compute the grand potential of the BCC and FCC structures, we need to solve the BdG equation

\[
\sum_{G'} (\mathcal{H}_{\Delta \delta \mu})_{G'G}(k) \phi_{G'}(k) = E(k) \phi_G(k),
\]

(26)
FIG. 4: The GL potential curves of the BCC structure for different values of $\bar{\eta}$ at $\delta \mu = \delta \mu_2 = 0.754 \Delta_0$. 

FIG. 5: The GL potential curves of the BCC structure for different values of $\bar{\eta}$ at the first-order phase transition point $\delta \mu = \delta \mu_*$. 

where the Hamiltonian matrix $(\mathcal{H}_{A,\delta \mu})_{G,G'}(\mathbf{k})$ is given by

$$
(\mathcal{H}_{A,\delta \mu})_{G,G'}(\mathbf{k}) = \begin{pmatrix}
(k + G| - \mu - \delta \mu)\delta_{G,G'}
& \Delta_{G-G'}

-(k + G| - \mu + \delta \mu)\delta_{G,G'}
& -(k + G| - \mu - \delta \mu)\delta_{G,G'}
\end{pmatrix}.
$$

The eigenstate $\phi_G$ includes two components $u_G$ and $v_G$ as usual in the BCS theory. We have

$$
\phi_G(\mathbf{k}) = \begin{pmatrix}
u_G(\mathbf{k})
u_G(\mathbf{k})\end{pmatrix}.
$$

We notice that $\delta \mu$ can be absorbed into the eigenvalues. The BdG equation can be rewritten as

$$
\sum_{G'}(\mathcal{H}_{A})_{G,G'}(\mathbf{k})\phi_G'(\mathbf{k}) = [E(\mathbf{k}) + \delta \mu] \phi_G(\mathbf{k}),
$$

where the Hamiltonian matrix $(\mathcal{H}_{A})_{G,G'}(\mathbf{k})$ reads

$$
(\mathcal{H}_{A})_{G,G'}(\mathbf{k}) = \begin{pmatrix}
(k + G| - \mu)\delta_{G,G'}
& \Delta_{G-G'}

-(k + G| - \mu - \delta \mu)\delta_{G,G'}
& -(k + G| - \mu + \delta \mu)\delta_{G,G'}
\end{pmatrix}.
$$

By using the fact $\Delta_{G-G'} = \Delta_{G'-G}$, we can show that: (1) The eigenvalues of $\mathcal{H}_A$ do not depend on the sign of $\Delta$; (2) If $\xi$ is an eigenvalue of $\mathcal{H}_A$, $-\xi$ must be another eigenvalue. Therefore, replacing the $\delta \mu$ by $-\delta \mu$ amounts to a replacement of the eigenvalue spectrum $\{E_i(\mathbf{k})\}$ by $\{-E_i(\mathbf{k})\}$. 


The Hamiltonian matrix has infinite dimensions. In practice, we make a symmetrical truncation $-D < l, m, n < D$. Then the BdG equation can be expressed as a matrix equation

$$
\mathbf{H} \begin{pmatrix} u \\ v \end{pmatrix} = \left( \begin{array}{cc} \mathbf{H}_{11} & \mathbf{H}_{12} \\ \mathbf{H}_{21} & \mathbf{H}_{22} \end{array} \right) \begin{pmatrix} u \\ v \end{pmatrix} = (E + \delta \mu) \begin{pmatrix} u \\ v \end{pmatrix},
$$

(31)

where $u$ and $v$ are $(2D + 1)^3$-dimensional vectors and $\mathbf{H}_{ij}$ are $(2D + 1)^3 \times (2D + 1)^3$ matrices. The matrices $\mathbf{H}_{ij}$ can be formally expressed as

$$
\mathbf{H}_{11}^{[l,m,n],[l',m',n']} = -\mathbf{H}_{22}^{[l,m,n],[l',m',n']} = \xi^{[l,m,n]} \delta_{l,l'} \delta_{m,m'} \delta_{n,n'},
$$

$$
\mathbf{H}_{12}^{[l,m,n],[l',m',n']} = \mathbf{H}_{21}^{[l,m,n],[l',m',n']} = \Delta^{[l-l',m-m',n-n']} = \Delta \mathbf{G} \mathbf{G}',
$$

(32)

where

$$
\xi^{[l,m,n]} = \left| k + \frac{2\pi}{a} (l x + m y + n z) \right| - \mu = \sqrt{k_x^2 + \frac{2\pi l^2}{a^2}} + \sqrt{k_y^2 + \frac{2\pi m^2}{a^2}} + \sqrt{k_z^2 + \frac{2\pi n^2}{a^2}} - \mu.
$$

(33)

Here the matrix index $[l, m, n]$ corresponds to the reciprocal lattice vector $\mathbf{G} = (2\pi/a)(l x + m y + n z)$. It shows that the blocks $\mathbf{H}_{11}$ and $\mathbf{H}_{22}$ are diagonal. The other two blocks $\mathbf{H}_{12}$ and $\mathbf{H}_{21}$ carry the information of the order parameter $\Delta$.

For a specific value of $D$, we can write down the explicit form of the vectors $u$ and $v$ and the matrices $\mathbf{H}_{ij}$. Here we use $D = 1$ as an example. The vectors $u$ and $v$ are 27-dimensional can be expressed as

$$
u = \begin{pmatrix} u_{[-1,-1]} \\ u_{[-1,0]} \\ u_{[-1,1]} \\ u_{[0,-1]} \\ u_{[0,0]} \\ u_{[0,1]} \\ u_{[1,-1]} \\ u_{[1,0]} \\ u_{[1,1]} \end{pmatrix}.$$

$$
u = \begin{pmatrix} v_{[-1,-1]} \\ v_{[-1,0]} \\ v_{[-1,1]} \\ v_{[0,-1]} \\ v_{[0,0]} \\ v_{[0,1]} \\ v_{[1,-1]} \\ v_{[1,0]} \\ v_{[1,1]} \end{pmatrix},
$$

(34)

where $u_{[l,m]}$ and $v_{[l,m]}$ are defined as

$$
u_{[l,m]} = \begin{pmatrix} u_{[l,m,-1]} \\ u_{[l,m,0]} \\ u_{[l,m,1]} \end{pmatrix}.$$

$$
u_{[l,m]} = \begin{pmatrix} v_{[l,m,-1]} \\ v_{[l,m,0]} \\ v_{[l,m,1]} \end{pmatrix}.
$$

(35)

In this representation, the off diagonal blocks $\mathbf{H}_{12}$ and $\mathbf{H}_{21}$ reads

$$
\mathbf{H}_{12} = \begin{pmatrix} \Delta_1 & \Delta_2 & 0 & \Delta_2 & 0 & 0 & 0 & 0 & 0 \\ \Delta_2 & \Delta_1 & \Delta_2 & 0 & \Delta_2 & 0 & 0 & 0 & 0 \\ 0 & \Delta_2 & \Delta_1 & 0 & \Delta_2 & 0 & 0 & 0 & 0 \\ \Delta_2 & 0 & 0 & \Delta_1 & \Delta_2 & 0 & \Delta_2 & 0 & 0 \\ 0 & \Delta_2 & 0 & \Delta_2 & \Delta_1 & \Delta_2 & 0 & 0 & 0 \\ 0 & 0 & \Delta_2 & 0 & \Delta_2 & \Delta_1 & 0 & 0 & \Delta_2 \\ 0 & 0 & 0 & \Delta_2 & 0 & \Delta_2 & \Delta_1 & \Delta_2 & 0 \\ 0 & 0 & 0 & 0 & \Delta_2 & 0 & \Delta_2 & \Delta_1 & \Delta_2 \\ 0 & 0 & 0 & 0 & 0 & \Delta_2 & \Delta_2 & \Delta_1 & \Delta_2 \end{pmatrix}.
$$

(36)

for BCC structure and

$$
\mathbf{H}_{12} = \begin{pmatrix} 0 & 0 & 0 & 0 & \Delta_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \Delta_1 & 0 & \Delta_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \Delta_1 & 0 & \Delta_1 & 0 & 0 & 0 \\ 0 & \Delta_1 & 0 & 0 & 0 & 0 & \Delta_1 & 0 & 0 \\ 0 & 0 & \Delta_1 & 0 & 0 & 0 & 0 & \Delta_1 & 0 \\ 0 & 0 & 0 & \Delta_1 & 0 & 0 & 0 & 0 & \Delta_1 \\ 0 & 0 & 0 & \Delta_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \Delta_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \Delta_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \Delta_1 & 0 & 0 \end{pmatrix}.
$$

(37)
for FCC structure. Here the blocks $\Lambda_1$ and $\Lambda_2$ are defined as

$$\Lambda_1 = \begin{pmatrix} 0 & \Delta & 0 \\ \Delta & 0 & \Delta \\ 0 & \Delta & 0 \end{pmatrix}, \quad \Lambda_2 = \begin{pmatrix} \Delta & 0 & 0 \\ 0 & \Delta & 0 \\ 0 & 0 & \Delta \end{pmatrix}. \quad (38)$$

The eigenvalues or the so-called band dispersion $E_{\lambda}(k)$ can be obtained by diagonalizing the $2(2D+1)^3 \times 2(2D+1)^3$ matrix $H$. In principle, $D$ should be large enough to achieve convergence. For realistic diagonalization, it is better to reduce the size of the matrix. Here we find that, with a proper rearrangement of the basis $\phi$ or after a similarity transformation, the matrix $H$ becomes block diagonal. We have

$$H \sim \begin{pmatrix} H_+ & 0 \\ 0 & H_- \end{pmatrix}, \quad (39)$$

where $H_+$ and $H_-$ are both $(2D+1)^3 \times (2D+1)^3$ matrices. The basis $\phi$ is now defined as

$$\phi = \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix}. \quad (40)$$

For $D = 1$, the 27-dimensional vectors $\phi_+$ and $\phi_-$ are given by

$$\phi_+ = \begin{pmatrix} u_{[-1,-1,-1]} \\ u_{[-1,-1,0]} \\ u_{[-1,-1,1]} \\ u_{[-1,0,-1]} \\ u_{[-1,0,0]} \\ u_{[-1,0,1]} \\ u_{[-1,1,-1]} \\ u_{[-1,1,0]} \\ u_{[-1,1,1]} \\ u_{[0,-1,-1]} \\ u_{[0,-1,0]} \\ u_{[0,-1,1]} \\ u_{[0,0,-1]} \\ u_{[0,0,0]} \\ u_{[0,0,1]} \\ u_{[0,1,-1]} \\ u_{[0,1,0]} \\ u_{[0,1,1]} \\ u_{[1,-1,-1]} \\ u_{[1,-1,0]} \\ u_{[1,-1,1]} \\ u_{[1,0,-1]} \\ u_{[1,0,0]} \\ u_{[1,0,1]} \end{pmatrix}, \quad \phi_- = \begin{pmatrix} u_{[-1,-1,-1]} \\ u_{[-1,-1,0]} \\ u_{[-1,-1,1]} \\ u_{[-1,0,-1]} \\ u_{[-1,0,0]} \\ u_{[-1,0,1]} \\ u_{[-1,1,-1]} \\ u_{[-1,1,0]} \\ u_{[-1,1,1]} \\ u_{[0,-1,-1]} \\ u_{[0,-1,1]} \\ u_{[0,0,-1]} \\ u_{[0,0,0]} \\ u_{[0,0,1]} \\ u_{[0,1,-1]} \\ u_{[0,1,0]} \\ u_{[0,1,1]} \\ u_{[1,-1,-1]} \\ u_{[1,-1,1]} \\ u_{[1,0,-1]} \\ u_{[1,0,0]} \\ u_{[1,0,1]} \end{pmatrix}, \quad (41)$$

which is just a proper rearrangement of the original basis given by (9) and (15). The matrices $H_+$ and $H_-$ can be expressed as

$$H_+ = \pm H_0 + H_{12}, \quad (42)$$

where $H_{12}$ is given by (13) or (17) and (18) for $D = 1$. $H_0$ is a diagonal matrix containing the kinetic energies. For $D = 1$ we have

$$H_0 = \text{diag}(\xi_{[-1,-1,-1]}, \xi_{[1,-1,0]}, \xi_{[-1,-1,1]}, \xi_{[0,0,0]}, \xi_{[-1,1,-1]}, \xi_{[1,1,0]}, \xi_{[-1,1,1]}). \quad (43)$$

It is easy to show that the eigenvalue spectra of $H_+$ and $H_-$ are dependent: If the eigenvalue spectrum of $H_+$ is given by $(\varepsilon_1(k))$, the eigenvalue spectrum of $H_-$ reads $[-\varepsilon_1(k)]$. Therefore, we only need to diagonalize the matrix $H_+$ or $H_-$. which has a dimension $(2D+1)^3$. Once the eigenvalue spectrum of $H_+$ is known, the eigenvalue spectrum of Hamiltonian matrix $\mathcal{H}_{\lambda,\mu}$ is given by $\{E_{\lambda}(k)\} = \{\varepsilon_1(k) - \partial \mu\} \cup \{-\varepsilon_1(k) - \partial \mu\}$. 


Calculation of the LO State

The calculation of the grand potential of the LO state is similar but much simpler than the 3D crystalline structures. The order parameter of the LO state can be expressed as

$$\Delta(z) = 2\Delta \cos(2qz).$$

(44)

It is periodic along the z direction with the periodicity $a = \pi / q$. So it can be decomposed into a discrete set of Fourier components,

$$\Delta(z) = \sum_n \Delta_n e^{2nqz},$$

(45)

where $n \in \mathbb{Z}$. The Fourier component $\Delta_n$ is given by

$$\Delta_n = \frac{1}{a} \int_0^a dz \Delta(z) e^{-2nqz} = \Delta (\delta_{n,1} + \delta_{n,-1}).$$

(46)

The BdG equation takes a similar form as the 3D structures. We have

$$\sum_n (\mathcal{H}_{\Delta,\delta\mu})_{n,n'}(\mathbf{k}) \phi_n(\mathbf{k}) = E(\mathbf{k}) \phi_n(\mathbf{k}),$$

(47)

where the Hamiltonian matrix $(\mathcal{H}_{\Delta,\delta\mu})_{n,n'}(\mathbf{k})$ is given by

$$(\mathcal{H}_{\Delta,\delta\mu})_{n,n'}(\mathbf{k}) = \begin{pmatrix} (\xi_n - \delta\mu)\delta_{n,n'} & \Delta_{n-n'} \\ \Delta_{n-n'} & -(\xi_n + \delta\mu)\delta_{n,n'} \end{pmatrix}$$

(48)

with

$$\xi_n = |k + 2nq| - \mu = \sqrt{k^2 + (kz + 2nq)^2} - \mu.$$  

(49)

We notice that only the motion in the z direction becomes quantized. The BZ for $k_z$ can be defined as $-\pi / a < k_z < \pi / a$ or $-q < k_z < q$. The eigenstate $\phi_n$ includes two components $u_n$ and $v_n$. We have

$$\phi_n(\mathbf{k}) = \begin{pmatrix} u_n(\mathbf{k}) \\ v_n(\mathbf{k}) \end{pmatrix}.$$  

(50)

The imbalance $\delta\mu$ can be absorbed into the eigenvalue. The BdG equation can be rewritten as

$$\sum_n (\mathcal{H}_{\Delta})_{n,n'}(\mathbf{k}) \phi_n(\mathbf{k}) = [E(\mathbf{k}) + \delta\mu] \phi_n(\mathbf{k}),$$

(51)

where the Hamiltonian matrix $(\mathcal{H}_{\Delta})_{n,n'}(\mathbf{k})$ reads

$$(\mathcal{H}_{\Delta})_{n,n'}(\mathbf{k}) = \begin{pmatrix} \xi_n\delta_{n,n'} & \Delta_{n-n'} \\ \Delta_{n-n'} & -\xi_{n}\delta_{n,n'} \end{pmatrix}.$$  

(52)

By using the fact $\Delta_{n-n'} = \Delta_{n'-n}$, we can show that: (1) The eigenvalues of $\mathcal{H}_{\Delta}$ do not depend on the sign of $\Delta$; (2) If $\varepsilon$ is an eigenvalue of $\mathcal{H}_{\Delta}$, $-\varepsilon$ must be another eigenvalue. Therefore, replacing the $\delta\mu$ by $-\delta\mu$ amounts to a replacement of the eigenvalue spectrum $\{E_{\varepsilon}(\mathbf{k})\}$ by $\{-E_{\varepsilon}(\mathbf{k})\}$.

After a truncation $-D < n < D$, the BdG equation can be expressed as a matrix equation

$$\mathbf{H} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} \mathbf{H}_{11} & \mathbf{H}_{12} \\ \mathbf{H}_{21} & \mathbf{H}_{22} \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = (E + \delta\mu) \begin{pmatrix} u \\ v \end{pmatrix},$$

(53)

where $u$ and $v$ are $(2D + 1)$-dimensional vectors and $\mathbf{H}_{ij}$ are $(2D + 1) \times (2D + 1)$ matrices. For a specific value of $D$, we can write down the explicit form of the vectors $u$ and $v$ and the matrices $\mathbf{H}_{ij}$. Here we use $D = 2$ as an example. The vectors $u$ and $v$ are 5-dimensional can be expressed as

$$u = \begin{pmatrix} u_{-2} \\ u_{-1} \\ u_0 \\ u_1 \\ u_2 \end{pmatrix}, \quad v = \begin{pmatrix} v_{-2} \\ v_{-1} \\ v_0 \\ v_1 \\ v_2 \end{pmatrix}.$$  

(54)
The matrices $H_{ij}$ can be explicitly written as

$$H_{11} = -H_{22} = \begin{pmatrix} \xi_{-2} & 0 & 0 & 0 \\ 0 & \xi_{-1} & 0 & 0 \\ 0 & 0 & \xi_0 & 0 \\ 0 & 0 & 0 & \xi_1 \\ 0 & 0 & 0 & \xi_2 \end{pmatrix}, \quad H_{12} = H_{21} = \begin{pmatrix} 0 & \Delta & 0 & 0 \\ \Delta & 0 & \Delta & 0 \\ 0 & \Delta & 0 & \Delta \\ 0 & 0 & \Delta & 0 \end{pmatrix}. \quad (55)$$

The eigenvalues $E_i(k)$ can be obtained by diagonalizing the $2(D + 1) \times 2(D + 1)$ matrix $H$. In principle, $D$ should be large enough to achieve convergence. For realistic diagonalization, it is better to reduce the size of the matrix. Here we find that, with a proper rearrangement of the basis $\phi$ or after a similarity transformation, the matrix $H$ becomes block diagonal. We have

$$H \sim \begin{pmatrix} H_{++} & 0 \\ 0 & H_{--} \end{pmatrix}, \quad (56)$$

where $H_{++}$ and $H_{--}$ are both $(2D + 1) \times (2D + 1)$ matrices. The basis $\phi$ is now defined as

$$\phi = \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix}. \quad (57)$$

For $D = 2$, the 5-dimensional vectors $\phi_+$ and $\phi_-$ are given by

$$\phi_+ = \begin{pmatrix} \mu_{-2} \\ \mu_{-1} \\ \mu_0 \\ \mu_1 \\ \mu_2 \end{pmatrix}, \quad \phi_- = \begin{pmatrix} \nu_{-2} \\ \nu_{-1} \\ \nu_0 \\ \nu_1 \\ \nu_2 \end{pmatrix}. \quad (58)$$

The matrices $H_{++}$ and $H_{--}$ can be expressed as

$$H_{++} = \pm H_0 + H_{12}. \quad (59)$$

$H_0$ is a diagonal matrix containing the kinetic energies. For $D = 2$ we have

$$H_0 = \text{diag}(\xi_{-2}, -\xi_{-1}, \xi_0, -\xi_1, \xi_2). \quad (60)$$

For general $D$, it is quite easy to write down the matrices $H_{++}$ and $H_{--}$. The eigenvalue spectra of $H_{++}$ and $H_{--}$ are dependent: If the eigenvalue spectrum of $H_{++}$ is given by $\{\varepsilon_{ij}(k)\}$, the eigenvalue spectrum of $H_{--}$ reads $\{-\varepsilon_{ij}(k)\}$. Therefore, we need only to diagonalize the matrix $H_{++}$ or $H_{--}$ which has a dimension $2D + 1$. Once the eigenvalue spectrum of $H_{++}$ is known, the eigenvalue spectrum of Hamiltonian matrix $H_{\delta \mu}$ is given by $\{E(k)\} = \{\varepsilon_{ij}(k) - \delta \mu\} \cup \{-\varepsilon_{ij}(k) - \delta \mu\}$.

In practice, we choose a sufficiently large $D$ and diagonalize the matrix $H_{++}$ or $H_{--}$ to obtain the eigenvalues $E_i(k)$. The thermodynamic potential of the LO state at zero temperature can be expressed as

$$\Omega_{LO} = \frac{\Delta^2}{2H} - 2 \int \frac{d^2k_\perp}{(2\pi)^2} \int_{BZ} \frac{dk_z}{2\pi} \sum_\Delta |E_i(k_\perp, k_z)|. \quad (61)$$

Similar Pauli-Villars-like regularization scheme should be applied finally. In Fig. 5(a), we show the grand potential of the LO state for $\Delta_0 = 80$ MeV. The grand potential for the self-consistent 1D modulation for $\Delta_0 = 80$ MeV was also reported in [3, 4]. We find that the results for the LO state and the self-consistent 1D modulation agrees with each other near the phase transition to the normal state. Near the BCS-LO transition point, the self-consistent 1D modulation has lower grand potential than the LO state. It was shown in [3] that the self-consistent 1D modulation forms a soliton lattice structure near the lower critical field, which lowers the grand potential of the system. Near the upper critical field the gap function becomes sinusoidal, and therefore the grand potentials of the LO state and the 1D modulation agree with each other. We notice that the phase transition from the LO state to the normal state is of first order, which is in contradiction to the prediction from the GL analysis. To understand the reason, we show in Fig. 5(b) the potential curve at $\delta \mu = 0.775 \Delta_0$ and at the optimal pair momentum $q = 1.1613 \delta \mu$. We find that the potential curve has two minima: a shallow minimum at $\Delta \approx 0.12 \Delta_0$ and a deep minimum at $\Delta \approx 0.44 \Delta_0$. Obviously, the shallow minimum is responsible for the GL theory which predicts a second-order phase transition. However, the deep global minimum, which cannot be captured by the GL theory up to the order $\Delta^6$, is responsible for the real first-order phase transition. Therefore, the LO state already shows the importance of the higher-order expansions in the GL theory.
The key problem in the numerical calculation is the diagonalization of the matrix $H_+$ or $H_-$ and obtaining all the eigenvalues. For BCC and FCC structures, we use a symmetrical truncation $-D < l, m, n < D$ with a large cutoff $D \in \mathbb{Z}^+$. However, the matrix size grows dramatically with increasing cutoff $D$, which makes the calculation infeasible because of not only the computing capability of current computing facilities but also the computing time and cost. Notice that we need to diagonalize the matrix $H_+$ for various values of the momentum $k$ in the BZ, the gap parameter $\Delta$, and the pair momentum $q$.

We first estimate the size of the cutoff $D$ needed for the convergence of the grand potential $\delta \Omega$. The matrix size $(2D + 1)^3$ and hence the computing time and cost grow dramatically with increasing $D$. The cutoff $D$ is related to the maximum momentum $k_{\text{max}}$ in each direction ($x, y,$ and $z$). We have

$$k_{\text{max}} = (2D + 1) \frac{\pi}{a},$$

This maximum momentum can be roughly estimated from the calculation of the LO state. For the LO state, the matrix size becomes $2D + 1$ and exact diagonalization is possible. The regime of $\delta \mu$ we are interested in is $\delta \mu/\Delta_0 \in [0.7 - 0.8]$ and the optimal pair momentum is located at $q \approx \delta \mu$. From the calculation of the LO state at $\Delta_0 \approx 100$ MeV, we find that $k_{\text{max}}$ must reach at least 5 GeV for convergence. Notice that we have $k_{\text{max}} = (2D + 1)q$ for BCC and $\sqrt{3}k_{\text{max}} = (2D + 1)q$ for FCC. Therefore, the cutoff $D$ for BCC can be estimated as $D \sim 35$, which corresponds to a matrix size $\sim 3 \times 10^5$. For FCC, the cutoff is even larger because of the factor $\sqrt{3}$. We have $D \sim 60$ for FCC, which corresponds to a matrix size $\sim 1.5 \times 10^6$. Notice that this is only a naive estimation. In practice, the cutoff needed for convergence may be smaller or larger. Exact diagonalization of such huge matrices to obtain all the eigenvalues are impossible with our current computing facility.

We therefore need a feasible scheme to evaluate the grand potential $\delta \Omega$. Notice that decreasing the value of $\Delta_0$ does not reduce the size of the matrices. In this case, even though $k_{\text{max}}$ becomes smaller, the pair momentum $q$ also gets smaller. Let us call an off-diagonal element $\Delta$ in $H_+$ or $H_-$ a “coupling”. Because our goal is to evaluate the grand potential $\delta \Omega$ rather than to know exactly all the band dispersions (eigenvalues), we may neglect a small amount of couplings to lower the size of the matrices. By neglecting this small amount of couplings, the huge matrix $H_+$ becomes block diagonal with each block having a much smaller size. In general, we expect that the omission of a small amount of couplings $\Delta$ induces only a perturbation to the grand potential $\delta \Omega$. We shall call this scheme small block method (SBM).

To be specific, the size of the small blocks in our calculation is $(2D + 1)^3$ with $d \in \mathbb{Z}^+$. In general, we have $d < D$. For symmetry reason, we require that the centers of these blocks are located at the reciprocal lattice vectors

$$G_{[n_x, n_y, n_z]} = (2d + 1) \frac{2\pi}{a} (n_x e_x + n_y e_y + n_z e_z)$$

with $n_x, n_y, n_z \in \mathbb{Z}$. This scheme makes the SBM feasible even though $(2D + 1)^3$ is not divisible by $(2D + 1)^3$. In practice, we first choose a large cutoff $D$ which is sufficient for convergence. By increasing the value of $d$, we find that the grand potential $\delta \Omega$ finally converges. In practice, if the grand potentials evaluated at several values of $d$, i.e., $d_0 - k, d_0 - k + 1, \ldots$, and $d_0 (k \in \mathbb{Z}^+)$, are very close to each other, we identify that the grand potential converges to its precise value from exact diagonalization. At the
converging value \( d = d_0 \), the block size \((2d_0 + 1)^3\) is normally much smaller than the total size \((2D + 1)^3\). This scheme makes the calculation feasible and also saves a lot of computing time and cost.

The matrices for the 3D structures are huge and cannot be written down here. For the sake of simplicity, let us use the LO state as a toy example for the SBM. In this case, the matrix size and the block size are \(2D + 1\) and \(2d + 1\), respectively. The centers of the blocks are located at the reciprocal lattice vectors \((2d + 1)2q_n\zeta\) with \(n_\zeta \in \mathbb{Z}\). For \(D = 10\), the matrix \(H_+\) reads

\[
\begin{pmatrix}
\epsilon_{+10} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\Delta & \epsilon_{+9} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \Delta & \epsilon_{+8} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \Delta & \epsilon_{+7} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \Delta & \epsilon_{+6} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \Delta & \epsilon_{+5} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{+4} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{+3} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{+2} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{+1} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_0 & \Delta & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-1} & \Delta & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-2} & \Delta & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-3} & \Delta & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-4} & \Delta & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-5} & \Delta \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-6} & \Delta \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-7} & \Delta \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-8} & \Delta \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-9} & \Delta \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-10} & \\
\end{pmatrix},
\]

where \(\epsilon_n = (-1)^n \sqrt{K^2_{\zeta} + (k_\zeta + 2nq_\zeta)^2} - \mu\). If we take \(d = 2\), we neglect the couplings \(\Delta\) in red. In this case, the matrix \(H_+\) is approximated as

\[
\begin{pmatrix}
\epsilon_{+10} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\Delta & \epsilon_{+9} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \Delta & \epsilon_{+8} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \Delta & \epsilon_{+7} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \Delta & \epsilon_{+6} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \Delta & \epsilon_{+5} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{+4} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{+3} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{+2} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{+1} & \Delta & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_0 & \Delta & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-1} & \Delta & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-2} & \Delta & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-3} & \Delta & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-4} & \Delta & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-5} & \Delta \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-6} & \Delta \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-7} & \Delta \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-8} & \Delta \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-9} & \Delta \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \Delta & \epsilon_{-10} & \\
\end{pmatrix},
\]

Therefore, by neglecting a small amount of couplings, we have made the large matrix \(H_+\) block-diagonal. Notice that this is only a toy example for the SBM. In practice, \(D = 10\) and \(d = 2\) is obviously not enough for convergence.

For the LO state, exact diagonalization of the matrices at \(q = \delta \mu\) is quite easy because the size of the matrices is \(2D + 1\). We
can therefore check the error induced by the SBM. The relative error induced by the SBM can be defined as

\[
R = \frac{\delta\Omega_{\text{SBM}} - \delta\Omega_{\text{EX}}}{\delta\Omega_{\text{EX}}},
\]

where \(\delta\Omega_{\text{SBM}}\) and \(\delta\Omega_{\text{EX}}\) are the grand potentials obtained from the SBM and exact diagonalization, respectively. In Fig. 7(a), we show a numerical example of the relative error for the LO state at \(\delta\mu/\Delta_0 = 0.77\) and \(q/\delta\mu = 1.16\). In the calculations, we use \(D = 50\) and \(d = 20\). We find that the relative error is very small, generally of order \(O(10^{-3})\). The slightly larger error around \(\Delta/\Delta_0 = 0.5\) is due to the fact that \(\delta\Omega\) itself is very small there. For the BCC structure, we are not able to check the relative error at \(q \approx \delta\mu\) because it is impossible to exactly diagonalize the matrices with a huge size \((2D + 1)^3\). However, for large \(q\), convergence can be reached at small \(D\) and exact diagonalization is possible. In Fig. 7(b), we show the relative error evaluated at \(\delta\mu/\Delta_0 = 0.75\) and \(q/\delta\mu = 4\). In this case, \(D = 9\) is enough for convergence and exact diagonalization is possible. We also use the SBM with \(d = 5\) to calculate the grand potential. We find that the relative error is also rather small, generally of order \(O(10^{-3})\). For pair momentum around \(q \approx \delta\mu\), we choose a sufficiently large cutoff \(D\) and increase the value of \(d\). We evaluate the grand potentials for various values of \(d\) (i.e., \(d_0 - k, d_0 - k + 1, \ldots, \) and \(d_0\)). If they are very close to each other, we identify that the grand potential converges. Then the grand potential \(\delta\Omega\) can be evaluated at \(d = d_0\).

[1] J. A. Bowers, K. Rajagopal, Phys. Rev. D66, 065002 (2002).
[2] R. Casalbuoni and G. Nardulli, Rev. Mod. Phys. 76, 263 (2004).
[3] D. Nickel and M. Buballa, Phys. Rev. D79, 054009 (2009).
[4] We have carefully checked that the numerical results of the grand potential \(\delta\Omega\) reported in [3] should be divided by a factor of 3.