Exact solution for finite center-of-mass momentum Cooper pairing

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Pair density waves (PDWs) are superconducting states formed by Cooper pairs of electrons containing a nonzero center-of-mass momentum. They are characterized by a spatially modulated order parameter and may occur in a variety of emerging quantum materials such as cuprates, transition-metal dichalcogenides (TMDs), and Kagome metals. Despite extensive theoretical and numerical studies seeking PDWs in a variety of lattices and interacting settings, there is currently no exact mechanism that spontaneously favors a modulated solution of the superconducting order parameter. Here, we study the problem of two electrons subject to an anisotropic attractive potential. We solve the two-body Schrödinger wave equation exactly to determine the pair binding energy as a function of the center-of-mass momentum. We find that a modulated (finite momentum) pair is favored over a homogeneous (zero momentum) solution above a critical, intermediate interaction strength. Hence our exact result justifies previous mean-field approximations that obtain modulated ground states at finite but large interactions. Using this insight from the exact two-body solution, we construct a variational many-body wave function and show that the conclusions of the two-body problem are robust in the many-body limit. Our results thus lay the theoretical and microscopic foundation for the existence of PDWs.

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I. INTRODUCTION

Cooper's proof [1] that the Fermi surface of a metal is unstable to a weak attractive potential between two quasiparticles laid the foundation for a subsequent comprehensive theory of superconductivity in elemental metals by Bardeen, Cooper, and Schrieffer [2]. The resulting bound state of the two quasiparticles, termed a Cooper pair, contains zero center-of-mass momentum and constitutes the basic building block of a superconductor. Recently the prospect of Cooper pairs with finite center-of-mass momentum has been raised and supported by several experimental observations in emerging quantum materials [3]. In time-reversal symmetric settings, such a phenomenon can manifest in pair density wave (PDW) phases—superconducting ground states defined by a spatially varying order parameter that breaks translation symmetries of the lattice and whose real-space average vanishes. A naïve implementation of Cooper's solution at infinitesimal coupling fails in this scenario and the following question arises: Is there an analog of the Cooper argument for finite center-of-mass momentum pairing? A resolution to this question would be a significant advancement toward uncovering the most basic microscopic ingredients driving Cooper pairing in PDWs. Here, we present an exact solution for the existence of such a two-body bound state with finite center-of-mass momentum in the presence of time-reversal symmetry as is relevant for a PDW. Widespread interest in PDWs has been triggered by independent experimental observations supporting short- or long-range PDW orders in different families of superconducting materials. These include the underdoped cuprates [4–16], Kagome metals [17], and transition-metal dichalcogenides [18]. However, despite concerted theoretical [19–38] and numerical [14,39–49] efforts, PDWs have not been found to occur as natural ground states [46–48]. At the current time, there is no known exact mechanism for why PDWs might be favored in some situations over other correlated phases including the homogeneous superconductor. Existing semianalytical approaches rely on mean-field/saddle point or effective field theoretical methods [24–26,33,34,37,38], which may at best be approximate away from weak coupling. Hence, a clear-cut exactly solvable model describing their origin from microscopic ingredients in a consistent manner is absent and has presented an open problem in superconductivity for decades. The question we address here is therefore an analog of the Cooper instability for a PDW, and our solution identifies its most basic microscopic building block from which other many-body solvable models can be constructed. While the contours of our derivation follow the original argument by Cooper and others [1,50,51]—two quasiparticles interacting via an effective attractive potential—we instead consider a problem where the quasiparticles, with a variable center-of-mass momentum $\mathbf{Q}$, interact through an effective anisotropic interaction. We then seek a solution to the Schrödinger wave

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equation for a two-particle bound state. Our main finding is the stability of a finite center-of-mass momentum ($\mathbf{Q} \neq 0$ mod $\mathbf{G}$; $\mathbf{G}$ being a reciprocal lattice vector) pair over a uniform solution with zero center-of-mass momentum ($\mathbf{Q} = 0$) above a critical interaction strength. Using the results of the two-body solution, we also construct a variational ansatz for the ground-state wave function of the many-body problem. An analysis of the superconducting pairing order parameter and free energy shows that the conclusions of the two-body solution also follow in the many-body limit. Our exact results thus provide a microscopic foundation for the existence of PDWs in a wide variety of superconducting materials and justify previous mean-field/weak coupling approximations that obtain modulated ground states at finite but large interactions [24–26,33,34]. In the remainder of the paper, we describe the effective interaction, derive an equation for the quasiparticle bound-state energy as a function of center-of-mass momentum, and finally discuss our results and conclusions.

II. INTERACTION

In his original work [1], Cooper assumed a constant (isotropic) interaction defined within an energy window set by the Debye frequency and zero otherwise. Here we instead choose an anisotropic interaction with nodes along certain directions in momentum space [35]. We motivate the momentum structure of the interaction so that the pairing form factor reduces to the d-wave (B_{1g}) symmetry in the zero center-of-mass momentum limit as seen, for example, in the cuprates [52]. For the $\mathbf{Q}$ dependence of the interaction, we consider Fourier transform of the pair hopping nematic operator relevant for d-wave charge fluctuations as observed in Raman scattering [53]. This implies that the incoming and outgoing momentum dependence of the pair potential is factorized as a product of two scalar form factors, $f_{\mathbf{kQ}}$ [35], which are functions of the two independent variables: the relative momentum $\mathbf{k}$ and center-of-mass momentum $\mathbf{Q}$. Writing out the interaction in momentum space, we have

$$V_{\mathbf{kk}'}(\mathbf{Q}) = \begin{cases} -V_0 f_{\mathbf{kQ}} f_{\mathbf{k}'\mathbf{Q}} & E_F \leqslant \epsilon_{\mathbf{k}} \leqslant \Lambda \\ 0 & \text{otherwise,} \end{cases} \tag{1}$$

with $V_0 > 0$, the form factor $f_{\mathbf{kQ}} \equiv (h_{\mathbf{k}-\mathbf{Q}/2} + h_{\mathbf{k}+\mathbf{Q}/2})$, E_F is the Fermi energy, $\epsilon_{\mathbf{k}}$ is the noninteracting dispersion, and $\sqrt{\Lambda}$ is an ultraviolet cutoff for the relative momentum $\mathbf{k}$ [35]. For the purposes of illustration, we choose the function $h(\mathbf{k}) = \sum_{n\in\mathbb{Z}} b_n(\cos nk_x - \cos nk_y)$ as is relevant for the cuprate square lattice; b_n is a constant. In the continuum, we use the appropriate expansion $h(\mathbf{k}) = \frac{1}{2\Lambda}\sum_{n\in\mathbb{Z}} n^2 b_n(k_y^2 - k_x^2)$. In two dimensions, a bound state is possible even without a Fermi surface in which case E_F can be set to zero. We will point it out explicitly when this is the case. Note that the interaction is constrained only in the relative momentum via $E_F \leqslant \epsilon_{\mathbf{k}} \leqslant \Lambda$ while the center-of-mass momentum $\mathbf{Q}$ is treated as a variational variable with respect to which the bound-state energy gain in maximized; the constraint itself is independent of the center-of-mass momentum. It is also worth mentioning that chosen momentum constraint is distinct from the interaction considered by Cooper, which is defined within a strict energy window above the Fermi energy.

III. COOPER PROBLEM FOR A PDW

We now use the two-body interaction $V_{\mathbf{k},\mathbf{k}'}(\mathbf{Q})$ in the two-body Schrödinger equation. For two electrons with kinetic energy $\epsilon_{\pm\mathbf{k}+\mathbf{Q}/2}$ and total center-of-mass momentum $\mathbf{Q}$, the momentum space two-electron Schrödinger equation is written as

$$(\epsilon_{\mathbf{k}+\mathbf{Q}/2} + \epsilon_{-\mathbf{k}+\mathbf{Q}/2} - E)g(\mathbf{k}) = -\sum_{\mathbf{k}'} V_{\mathbf{kk}'}(\mathbf{Q})g(\mathbf{k}').$$

The wave vector $\mathbf{k}$ ($\mathbf{Q}$) is the Fourier transform variable of the relative (center-of-mass) position coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ ($\mathbf{R} = \mathbf{r}_1 + \mathbf{r}_2$) with $\mathbf{r}_i$ being the position vector of the ith electron. The variable E is the eigenenergy whose functional form with respect to $\mathbf{Q}$ is to be determined. $g(\mathbf{k})$ is the Fourier component of the spatial part of the total wave function that depends on the relative position $\mathbf{r}$. To define this function more precisely, we denote the two-particle wave function as $\Psi(\mathbf{r}_1, \uparrow, \mathbf{r}_2, \downarrow)$ and decompose it into the spatial (ψ) and spin components (η) as $\Psi(\mathbf{r}_1, \uparrow, \mathbf{r}_2, \downarrow) = \psi(\mathbf{r}_1, \mathbf{r}_2)\eta_s(\uparrow, \downarrow)$. Here η_s is a spin singlet between the two electrons. For the spatial component of the wave function, we make the ansatz for a single wave vector $\mathbf{Q}$ as $\psi(\mathbf{r}_1, \mathbf{r}_2) = \Phi(\mathbf{r})e^{i\mathbf{Q}\cdot\mathbf{R}}$. Here $\Phi(\mathbf{r})$ depends only on the relative coordinate $\mathbf{r}$. Fourier decomposition of the function $\Phi(\mathbf{r})$ defines the function $g(\mathbf{k})$ as $\Phi(\mathbf{r}) = \frac{1}{\sqrt{v}}\sum_{\mathbf{k}} g(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}$ where v is the normalization volume. Substituting the interaction Eq. (1) into the momentum space Schrödinger wave equation Eq. (2) and using the factorization property of the interaction (see Appendix A), we obtain the condition

$$1 = |V_0| \sum_{\mathbf{k}} \left[\frac{f_{\mathbf{k},\mathbf{Q}}^2}{-E + \epsilon_{\mathbf{k}+\mathbf{Q}/2} + \epsilon_{-\mathbf{k}+\mathbf{Q}/2}} \right] \equiv F(E). \tag{2}$$

We can now solve Eq. (2) for the binding energy $E(\mathbf{Q})$. For the purposes of this discussion and relevant to the materials discussed above, we restrict our calculations to two dimensions. Generalization to three dimensions can be done readily.

IV. CONTINUUM CASE

We begin with the case of a continuum dispersion ($\frac{\hbar^2}{2m} = 1$; m is the bare electron mass) $\epsilon_{\mathbf{k}} = k^2$ where $k = |\mathbf{k}|$ and the density of states per spin is $\nu = \frac{1}{4\pi}$. For the moment, we set the Fermi energy to zero and integrate Eq. (2) over all allowed $\mathbf{k}$ such that only the lowest harmonic ($n = 1$) in the interaction is nonzero within the window $0 \leqslant k^2 \leqslant \Lambda$. A plot of $E(\mathbf{Q})$ appears in Fig. 1 for $\nu V_0 = 4/4\pi$. For the case when the interaction is isotropic with $f_{\mathbf{k},\mathbf{Q}}^2 = 1$ (s-wave scenario), the minimum of $E(\mathbf{Q})$ occurs at $\mathbf{Q} = 0$. Hence, Cooper pairs with zero center-of-mass momentum are stabilized and any finite momentum pairing reduces the binding energy of the pair. In this scenario, the homogeneous superconductor is favorable. For the case when the interaction is anisotropic with $f_{\mathbf{k},\mathbf{Q}}^2$ defined in Eq. (1), the homogeneous solution becomes destabilized (Fig. 1, bottom panel). While the binding energy continues to be suppressed along the diagonal (nodal) directions, the Cooper pairs acquire an unbounded gain in binding energy along the horizontal (antinodal) directions by taking on arbitrarily large center-of-mass momenta. Since, in the continuum, such arbitrarily large center-of-mass momentum

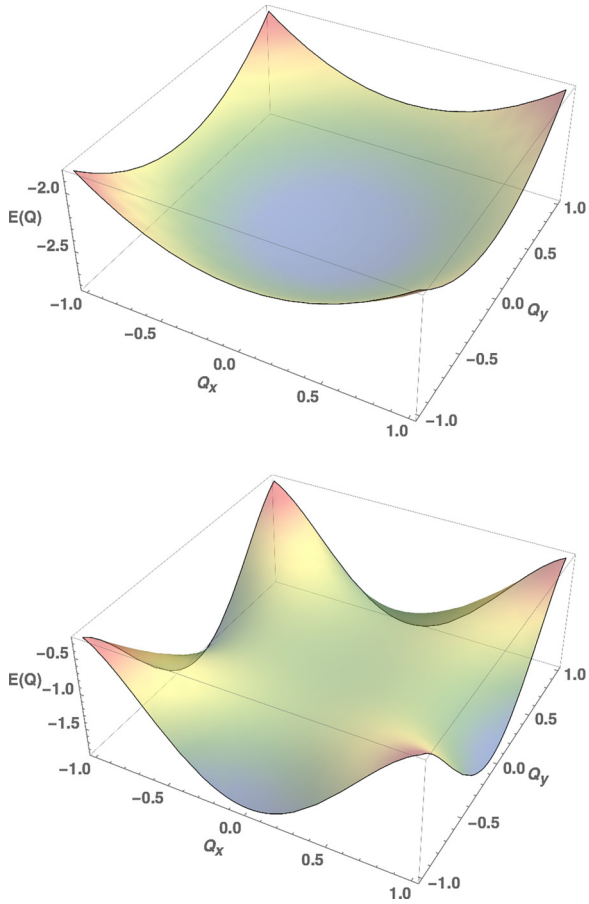

FIG. 1. Binding energy E as a function of momentum $\mathbf{Q}$ for isotropic s-wave (top) and anisotropic d-wave (bottom) interactions for a quadratic (continuum) dispersion. The interaction is fixed at $\nu V_0 = 4/4\pi$. The momenta are specified in units of $\sqrt{\Lambda}$ although they are unbounded in magnitude.

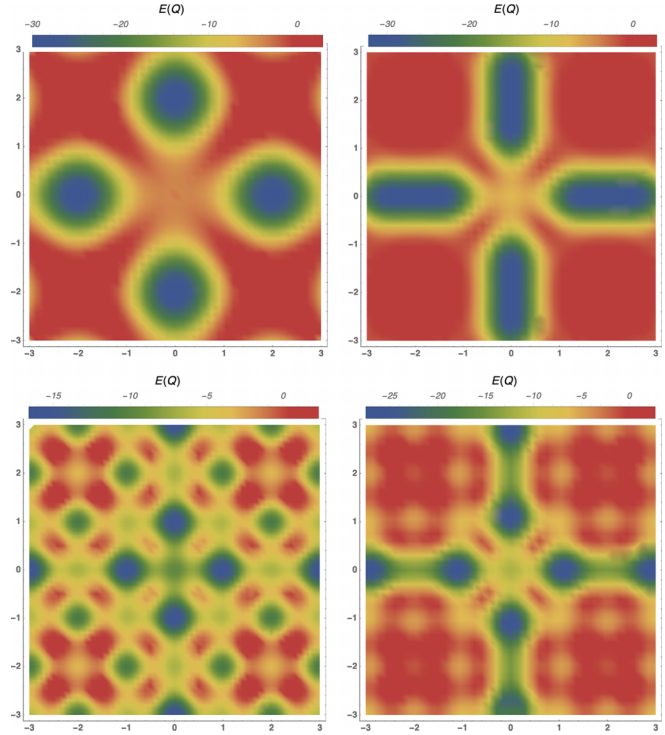

FIG. 2. Color density plots of the binding energy on a lattice as a function of $\mathbf{Q} = (Q_x, Q_y)$ (in units of π/a) for various d-wave harmonics. (Clockwise from top left) $(b_1, b_2) = (1, 0), (1, 0.5), (0.5, 1), (0, 1)$. We have set $t = 1$, $\nu V_0 = 30/2\pi$, and $\Lambda/W = 0.125$. The minimum continuously shifts from $(\pm 2\pi, 0), (0, \pm 2\pi)$ to $(\pm\pi, 0), (0, \pm\pi)$.

values are permitted, a stable minimum at finite and bounded $\mathbf{Q}$ does not exist. Even on a lattice where the binding energy is finite and periodic, as we will see below, a nontrivial and finite center-of-mass pairing is not guaranteed. This is because the binding energy minimum can, in principle, occur for a $\mathbf{Q}$ located at a reciprocal lattice vector. Nevertheless, such a runaway binding energy is a strong indicator of nonhomogeneous and modulated pairing, and understanding the stability of such solutions requires a background lattice.

Before we discuss the lattice case below, a few remarks are in order. Note that the interaction chosen in Eq. (1) has a sharp ultraviolet cutoff in momentum at $\sqrt{\Lambda}$; however, a smoothly varying interaction can also destabilize the homogeneous solution as long as it is dominant within the scale $\sqrt{\Lambda}$. Moreover, the aforementioned results in two dimensions are robust to the inclusion of a nonzero Fermi momentum within the integration limits appearing in Eq. (2). Finally, while the existence of an ultraviolet cutoff aids the finite-$\mathbf{Q}$ analysis, it is the nontriviality of the anisotropic interaction that really drives the destabilization of the homogeneous pairing solution and not the nature of the chosen cutoff (see Appendix D and Appendix E for an approximate formula of the binding energy where this is explicit). This can also be evidenced by the fact that the same choice of cutoff does not destabilize the homogeneous solution for a fully isotropic interaction.

V. LATTICE CASE

In the previous section we showed that, in continuum, the homogeneous pairing solution can become unstable to an anisotropic attractive interaction of the form appearing in Eq. (1), with a runaway binding energy along the antinodal direction. We now examine the stability of the finite-$\mathbf{Q}$ phase in the presence of a lattice. We take the example of a square lattice with a dispersion $\epsilon_{\mathbf{k}} = -t(\cos k_x + \cos k_y)$ with $t = 1$ and a bandwidth $W = 4t$. The Brillouin zone extends from $[-\pi, \pi]$ in the k_x and k_y directions. For the function $h(\mathbf{k})$ appearing in the interaction, we consider the two lowest d-wave harmonics $n = 1, 2$ with $\nu V_0 = 30/2\pi$ and $\Lambda/W = 0.125$. Figure 2 shows a density plot of the binding energy as a function of the center-of-mass momentum $\mathbf{Q}$ for various values of (b_1, b_2). The 4π periodicity of the binding energy with respect to $\mathbf{Q}$ is set by the definition of the momentum shift in Eqs. (1), (2), which in our case is $\pm\mathbf{Q}/2$. With only the lowest d-wave harmonic $(b_1, b_2) = (1, 0)$ (top left), the minimum occurs at $\mathbf{Q} = (\pm 2\pi, 0), (0, \pm 2\pi)$, which are reciprocal lattice vectors of the square lattice. On the other hand, with only the second d-wave harmonic $(b_1, b_2) = (0, 1)$ (bottom left), the minimum occurs at $\mathbf{Q} = (\pm\pi, 0), (0, \pm\pi)$ signaling a stable (nontrivial) finite momentum pairing instability. For intermediate values of (b_1, b_2), the minima continuously shift

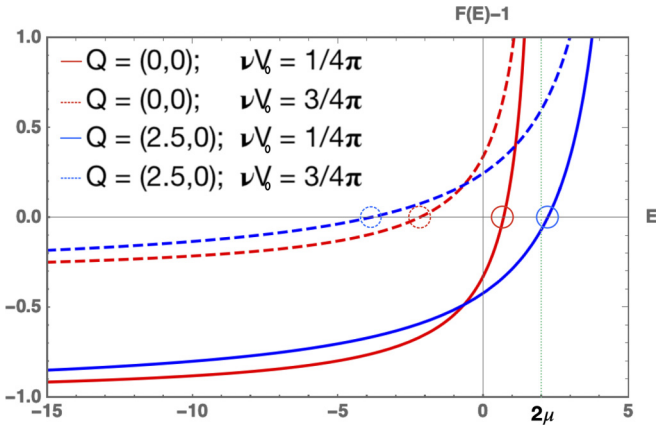

FIG. 3. Plots of the function $F(E)-1$ with binding energy E for two values of $\nu V_0 = 1/4\pi, 3/4\pi$ and two values of $\mathbf{Q} = (0,0), (2.5,0)$. The dotted green line denotes 2μ and zeros of $F(E)-1$ (solid and dashed circles) denote two-body bound-state values. For small (large) νV_0, $\mathbf{Q}=0$ ($\mathbf{Q}\neq 0$) solution has a greater binding energy with respect to 2μ.

between the two momenta (right panels). We also note that the nature of the solution depends on the existence of a cutoff Λ. This dependence is discussed in Appendix F.

VI. DEPENDENCE ON INTERACTION STRENGTH

We now address the dependence of the finite-$\mathbf{Q}$ transition on the interaction strength V_0. We show that for a given ratio Λ/W, finite momentum pairs are stabilized only above a critical value of νV_{0c}. We choose the continuum case for simplicity of illustration, but analogous arguments hold in the presence of a lattice. In the case of an isotropic s-wave pair potential, it is well known that even an infinitesimally small interaction (νV_0) can drive Cooper pairing with zero center-of-mass momentum. It is now established that a similar result holds for the uniform $\mathbf{Q}=0$ d-wave superconductor as well. This fact suggests that for weak enough interactions, the finite-$\mathbf{Q}$ pairing gives way to homogeneous $\mathbf{Q}=0$ pairing for weak enough νV_0. To confirm this, we show in Fig. 3 a plot of $F(E)-1$ with binding energy E where $F(E)$ is defined in Eq. (2). We have chosen a Fermi energy with $\mu=1$ and pairing within a narrow window $\mu \pm 0.2$. A zero of the equation $F(E)-1$ with $E<2\mu$ denotes pair binding. Here, an infinitesimally small νV_0, or any interaction value below a critical intermediate value $\nu V_{0c} \simeq 2/4\pi$ (solid curves in Fig. 3), stabilizes a uniform d-wave superconductor [see also Appendixes B and C for recovering the binding energy and instability temperature of a uniform d-wave superconductor from Eq. (2)]. Finite momentum pairing in this limit acts to reduce the pair binding energy and is hence less favored. However, above the critical intermediate interaction νV_{0c}, finite momentum pairs [dashed curves in Fig. 3 with $\mathbf{Q}=(\pm 2.5,0),(0,\pm 2.5)$] gain more in pair binding energy than the uniform pairs. This exact result leads to the stability of finite momentum pairing over uniform pairing at intermediate couplings.

VII. VARIATIONAL WAVE FUNCTION

Using these insights from the exact two-body solution, we have also constructed a variational many-body wave function and calculate the free energy and superconducting gap as a function of the center-of-mass momentum. A zero-temperature analysis of the energy shows that the conclusions of the two-body problem are robust in the many-body limit (see Appendixes G and H).

VIII. DISCUSSIONS AND CONCLUSIONS

We presented an exact solution to a two-body Schrödinger wave equation that demonstrates the stability of a finite center-of-mass momentum Cooper pair over a homogeneous (zero momentum) d-wave pair. To our knowledge, there is no such exact mechanism for why modulated pairing is favored over a homogeneous superconductor in the presence of time-reversal symmetry. Several semianalytical approaches that have been discussed so far rely on mean-field/saddle point or effective field theoretical methods [24–26,33,34,38], which may be only approximate away from infinitesimal coupling. This is despite widespread experimental evidence for fluctuating and static pair density waves in cuprates, Kagome metals, and transition-metal dichalcogenides.

The problem we defined here consists of two electrons subject to an anisotropic d-wave attractive potential dominant over a certain energy window. Above a critical, intermediate, value of the interaction strength, nonzero center-of-mass momentum Cooper pairs save more binding energy in comparison with the homogeneous solution, hence stabilizing Cooper pairs of a PDW. The solution we provide in this paper is, therefore, an analog to the Cooper argument for a time-reversal symmetry preserving fluctuating or static PDW. From our exact solution we see that, while the critical value of interaction for the finite momentum transition does not occur at infinitesimally small interactions, one does not necessarily require very strong couplings to achieve such a ground state. Hence our work provides a sound justification for existing mean-field/saddle point-based solutions [24–26,33,34,38]. We have further demonstrated that these conclusions hold even in a many-body setting by explicitly evaluating the nonhomogeneous superconducting gap and free energy using a BCS-like variational wave function ansatz for a PDW.

The stable finite momentum solution found here requires an unconventional pairing interaction [54] and cannot occur for isotropic s-wave interactions. In the latter case, Cooper pairs are local, and must hence be uniform with a nodeless superconducting ground state. Unconventional pairs, on the other hand, have nontrivial internal structure and are extended in real space [27]. This allows the ground state to stabilize finite momentum pairs with a nodal gap structure. Further, we do not rule out finite momentum pairing solutions in anisotropic s-wave order parameters, a problem left for future work. The aforementioned properties provide a guiding principle to search for PDWs in superconductors with unconventional order parameters. Our result thus sets the stage for further analytical and numerical exploration of these

intriguing phases of matter in correlated superconductors with unconventional pairing states.

Note added. Recently, a paper appeared demonstrating evidence of PDWs in an unconventional superconductor UTe_2 [55].

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APPENDIX A: DERIVING EQ. (1)

Substituting the spatial component of the wave function into the Schrödinger wave equation and writing in terms of Fourier components, we have

$$(\epsilon_{\mathbf{k}+\mathbf{Q}/2}+\epsilon_{-\mathbf{k}+\mathbf{Q}/2}-E)g(\mathbf{k})=-\sum_{\mathbf{k}'}V_{\mathbf{k}\mathbf{k}'}(\mathbf{Q})g(\mathbf{k}'), \quad \text{(A1)}$$

where $V_{\mathbf{k},\mathbf{k}'}$ are the Fourier components of the two-body interaction, which we assume to be separable of the form $V_{\mathbf{k},\mathbf{k}'}(\mathbf{Q})=f_{\mathbf{k},\mathbf{Q}}f_{\mathbf{k}',\mathbf{Q}}$. For the purposes of our discussion, we choose $f_{\mathbf{k},\mathbf{Q}}\equiv\frac{h_{\mathbf{k}-\mathbf{Q}/2}+h_{\mathbf{k}+\mathbf{Q}/2}}{2}$ where $h_{\mathbf{k}}$ is the B_{1g} d-wave form factor.

We can now solve for $g(\mathbf{k})$ we have

$$g(\mathbf{k})=\frac{\sum_{\mathbf{k}'}V_{\mathbf{k}\mathbf{k}'}(\mathbf{Q})g(\mathbf{k}')}{(-\epsilon_{\mathbf{k}+\mathbf{Q}/2}-\epsilon_{-\mathbf{k}+\mathbf{Q}/2}+E)}. \quad \text{(A2)}$$

Multiplying both sides with $V_{\mathbf{k},\mathbf{k}_1}(\mathbf{Q})$ and summing to over $\mathbf{k}$ simplifies the expression. Noting that the interaction $V_{\mathbf{k},\mathbf{k}'}(\mathbf{Q})$ is assumed to be factorizable, momentum summations on the left- and right-hand sides cancel. Assuming a negative (attractive) potential strength $-|V_0|$, the Eq. (A2) above reduces to

$$1=|V_0|\sum_{\mathbf{k}}\left[\frac{f^2_{\mathbf{k},\mathbf{Q}}}{-E+\epsilon_{\mathbf{k}+\mathbf{Q}/2}+\epsilon_{-\mathbf{k}+\mathbf{Q}/2}}\right]. \quad \text{(A3)}$$

We can now solve Eq. (A3) for the dispersion of binding energy $E(\mathbf{Q})$.

APPENDIX B: BINDING ENERGY OF HOMOGENEOUS d-WAVE SUPERCONDUCTOR

As we saw in the main text, for weak enough coupling V_0 in Eq. (2), the homogeneous $\mathbf{Q}=0$ solution is stable. Here we show that such a solution is exactly the conventional BCS d-wave superconductor. To prove this, we demonstrate that the $\mathbf{Q}=0$ solution to Eq. (2) can occur at infinitesimally small coupling strength V_0. We begin by converting Eq. (2) at $\mathbf{Q}=0$ into an energy integral that is nonzero only over a narrow energy window Ω around μ:

$$\frac{1}{|\bar{V}_0|}=2\int_{\bar{\mu}}^{\bar{\mu}+\bar{\Omega}}\frac{(\bar{\xi}+\bar{\mu})^2 d\bar{\xi}}{-\bar{E}+2\bar{\xi}}. \quad \text{(B1)}$$

Here the bar on top of each variable denotes normalization with respect to some high-energy scale. The integral above can be performed to yield a nonlinear equation for $\bar{E}$ given by

$$\frac{1}{|\bar{V}_0|}=\frac{1}{2}\Bigg[\bar{\Omega}(\bar{E}+6\bar{\mu}+\bar{\Omega}) + (\bar{E}+2\bar{\mu})^2\tanh\left(\frac{\bar{\Omega}}{-\bar{E}+2\bar{\mu}+\bar{\Omega}}\right)\Bigg]. \quad \text{(B2)}$$

This equation can be solved for $E<2\mu$ and a solution exists for infinitesimally small $|V_0|$. Hence we recover the binding energy of a conventional homogeneous d-wave superconductor.

APPENDIX C: INSTABILITY TEMPERATURE T_i OF HOMOGENEOUS d-WAVE SUPERCONDUCTOR

Here we calculate the instability temperature T_i for the homogeneous Cooper pair solution of Eq. (2) and show that we can recover the weak-coupling BCS-like formula. This can be done by taking the $\mathbf{Q}\to 0$ limit of the finite temperature pair susceptibility using the same form factor appearing in Eq. (2). For a large and positive μ (large Fermi surface) the static zero momentum pair susceptibility is given by

$$\Pi(\mathbf{q}\to 0,\omega=0)=\frac{1}{\beta\pi\Lambda^3}\sum_{\epsilon_n}\int_0^{\Lambda}\frac{4\pi k^5 dk}{(k^2-\mu)^2+\epsilon_n^2}, \quad \text{(C1)}$$

where Λ is an interaction cutoff, β the inverse temperature, and ϵ_n is the fermionic Matsubara frequency. Performing the Matsubara sum yields

$$\Pi(\mathbf{q}\to 0,\omega=0)=\frac{1}{\beta\pi\Lambda^3}\int_0^{\Lambda}4\pi k^5 dk\frac{\tanh\left(\frac{k^2-\mu}{2T}\right)}{2(k^2-\mu)T}. \quad \text{(C2)}$$

The instability temperature T_i (which equals the coherence temperature T_c at weak coupling) can be solved by setting $\Pi(\mathbf{q}\to 0,\omega=0)|_{T=T_i}-|V_0|^{-1}=0$. The nonlinear equation can be solved for T_i (for infinitesimal $|V_0|$) and takes the approximate BCS-like form

$$T_i\simeq\frac{\Lambda}{4}\exp\left[\frac{-1}{\pi\nu|V_0|}\right]. \quad \text{(C3)}$$

APPENDIX D: APPROXIMATE $E(\mathbf{Q})$ FOR Q ALONG ANTINODAL DIRECTION

Here we derive an approximate formula for the binding energy $E(\mathbf{Q})$ when $\mathbf{Q}$ is along the antinodal direction [$\mathbf{Q} = (\pm q, 0), (0, \pm q)$]. Substituting for $\mathbf{Q} = (q, 0)$ and neglecting the q dependence of the denominators (this is a good approximation for large enough q), we get

$$F(E) \simeq -\frac{|V_0|}{2\Lambda^3}\int_{\sqrt{2\mu}}^{\sqrt{2\mu+\Omega}} \frac{k(8k^4+q^4)}{E-2k^2+2\mu}dk. \tag{D1}$$

The integral above can be performed exactly and solved for $E(q)$ with $\Omega > 0$. For small Ω and above the critical $|V_0|$ where zero momentum solution is unstable, the expression for $E(q)$ takes an illuminating form

$$\bar{E}(q) \simeq 2\bar{\mu} - \tfrac{1}{4}|\bar{V}_0|(\bar{q}^4 + 32\bar{\mu}^2)\bar{\Omega}, \tag{D2}$$

where all quantities are dimensionless and normalized by the appropriate factor of Λ. The expression above shows that a zero momentum solution gives rise to a finite momentum solution. The finite momentum is cut off for large q either by the energy cutoff or the lattice and the energy gain is thus bounded from below.

APPENDIX E: APPROXIMATE $E(\mathbf{Q})$ FOR Q ALONG ANTINODAL DIRECTION

$E(\mathbf{Q})$ for $\mathbf{Q}$ along the nodal points. When $\mathbf{Q}$ is along the nodal direction, i.e., [$\mathbf{Q} = (\pm q, \pm q), (\pm q, \mp q)$], finite momentum pairs always reduce the gain pair binding energy; hence, they are unstable in comparison to the homogeneous d-wave superconductor. This can be seen readily by noting that the form factor in the interaction is independent of $\mathbf{Q}$ along the nodal regions; that is, $f_{\mathbf{k},\mathbf{Q}} = f_{\mathbf{k},0}$ along the diagonals. The remaining $\mathbf{Q}$ dependence of $F(E)$ occurs only in its denominator like in the s-wave case. Hence, finite momentum pairs always cost energy along the diagonal direction.

APPENDIX F: ROLE OF CUTOFF

The presence of a lattice also offers an avenue to examine the role of the cutoff Λ on the binding energy landscape. Figure 4 shows a density plot of the binding energy $E(\mathbf{Q})$ throughout the Brillouin zone for two values of the ratio Λ/W. The interaction parameter is fixed as $\nu V_0 \simeq 30/2\pi$ for the second d-wave harmonic and zero otherwise. For the case when the interaction window is a large fraction of the bandwidth, the minimum of $E(\mathbf{Q})$ occurs at $\mathbf{Q} = 0$. However, upon reducing the interaction window, there is a transition into a finite-$\mathbf{Q}$ phase where the minimum occurs at the edges of the Brillouin zone at $\mathbf{Q} = (\pm\pi, 0), (0, \pm\pi)$. The transition point is nonuniversal and, for the chosen interaction parameter values, occurs at around $\Lambda/W \sim 0.2$ where the local minima at the Brillouin zone edges is equal to that at the center. At this value, there is a first-order transition to the finite-$\mathbf{Q}$ phase as a function of Λ/W. Moreover, the cutoff chosen can be a smooth function of energy without qualitatively affecting the transition.

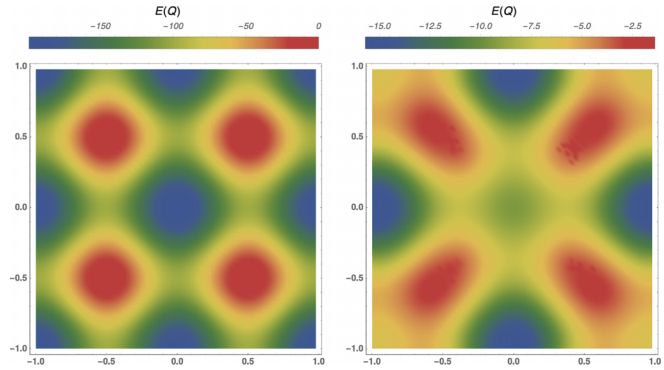

FIG. 4. Binding energy E as a function of momentum $\mathbf{Q}$ (units of π/a) for second harmonic anisotropic (d-wave) interactions on a lattice as a function of interaction cutoffs. Left and right panels correspond to $\Lambda/W = 1.0, 0.125$ respectively. The interaction parameter is set at $\nu V_0 = 30/2\pi$.

APPENDIX G: VARIATIONAL WAVE FUNCTION

The conclusions of the two-body problem can be readily generalized to a many-body setting. To do this, we use the BCS variational wave function approach to evaluate and minimize the superconducting contribution to the free energy. In addition to the usual BCS-like variational parameters, we introduce the center-of-mass momentum coordinate $\mathbf{Q}$ as another variational parameter. A free energy minimum away from $\mathbf{Q} = 0$ signals a transition to a many-body PDW phase. We begin the analysis by writing the total Hamiltonian in second quantized notation

$$\begin{aligned}\mathscr{H} &= \sum_{\mathbf{k}\sigma}\xi_{\mathbf{k}}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} + \mathscr{H}_I \\ \mathscr{H}_I &= \sum_{\mathbf{k}\mathbf{k}'\mathbf{Q}} V_{\mathbf{k}\mathbf{k}'}(\mathbf{Q})c^{\dagger}_{\mathbf{k}+\mathbf{Q}/2\uparrow}c^{\dagger}_{-\mathbf{k}+\mathbf{Q}/2\downarrow}c_{-\mathbf{k}'+\mathbf{Q}/2\downarrow}c_{\mathbf{k}'+\mathbf{Q}/2\uparrow},\end{aligned} \tag{G1}$$

where $\xi_{\mathbf{k}}$ and $V_{\mathbf{k}\mathbf{k}'}(\mathbf{Q})$ are the quasiparticle energy and interaction, respectively, $c^{\dagger}_{\mathbf{k}\sigma}$ creates a quasiparticle with momentum $\mathbf{k}$ and spin σ, $c^{\dagger}_{\mathbf{k}+\mathbf{Q}/2\,\sigma}c^{\dagger}_{-\mathbf{k}+\mathbf{Q}/2\,\bar{\sigma}}$ creates a pair of spin-singlet quasiparticles with relative momentum $\mathbf{k}$ and center-of-mass momentum $\mathbf{Q}$ ($\bar{\sigma}$ is the spin-flip projection). We choose a variational ansatz for the PDW wave function with a single wave vector $\mathbf{Q}$ given by

$$|\Psi_{\mathrm{PDW}}\rangle = \prod_{\mathbf{k}=\mathbf{k}_1}^{\mathbf{k}_M}(u_{\mathbf{k}}(\mathbf{Q}) + v_{\mathbf{k}}(\mathbf{Q})c^{\dagger}_{\mathbf{k}+\mathbf{Q}/2\uparrow}c^{\dagger}_{-\mathbf{k}+\mathbf{Q}/2\downarrow})|0\rangle. \tag{G2}$$

Here $v(\mathbf{Q})$ and $u(\mathbf{Q})$ are variational parameters along with the center-of-mass momentum $\mathbf{Q}$ that must be determined by minimizing the free energy (see next section for details of derivation), $|0\rangle$ is the vacuum state with no particles, and $\mathbf{k}_1..\mathbf{k}_M$ are the momentum values in the band. The zero-temperature free energy of the superconducting phase $E(\mathbf{Q})_S = \langle\Psi_{\mathrm{PDW}}|\mathscr{H}|\Psi_{\mathrm{PDW}}\rangle$ is given by (see next section for details of derivation)

$$E(\mathbf{Q})_S = \frac{1}{2}\sum_{\mathbf{k}}\bar{\xi}_{\mathbf{k}}(\mathbf{Q})\left[1 - \frac{\bar{\xi}_{\mathbf{k}}(\mathbf{Q})}{E_{\mathbf{k}}(\mathbf{Q})}\right] - \frac{4\bar{\Delta}(\mathbf{Q})^2}{V_0}, \tag{G3}$$

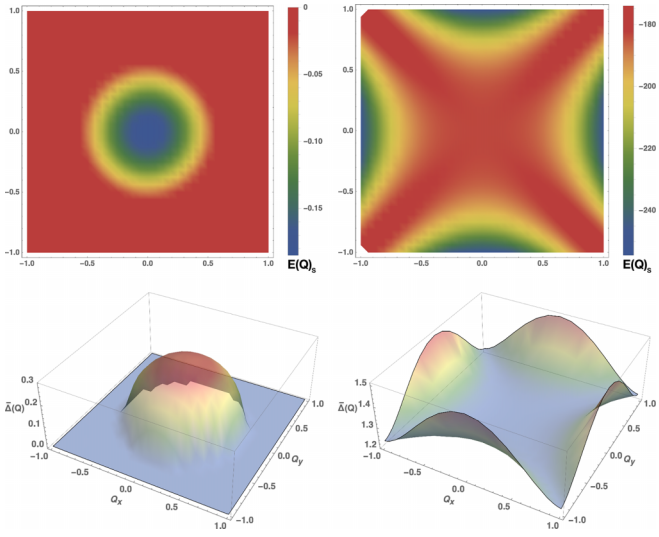

FIG. 5. (Top row) Plots of the free energy $E(\mathbf{Q})_S$ of the superconducting state as a function of center-of-mass momentum $\mathbf{Q}$ (units $\sqrt{\Lambda}$) for isotropic (left) and anisotropic (right) interactions. (Bottom row) Nonhomogeneous order parameter $\bar{\Delta}(\mathbf{Q})$ as a function of $\mathbf{Q}$ for isotropic (left) and anisotropic (right) interactions. The chemical potential is set to $\mu = 1$ and the interaction parameter is $\nu V_0 = 4/4\pi$.

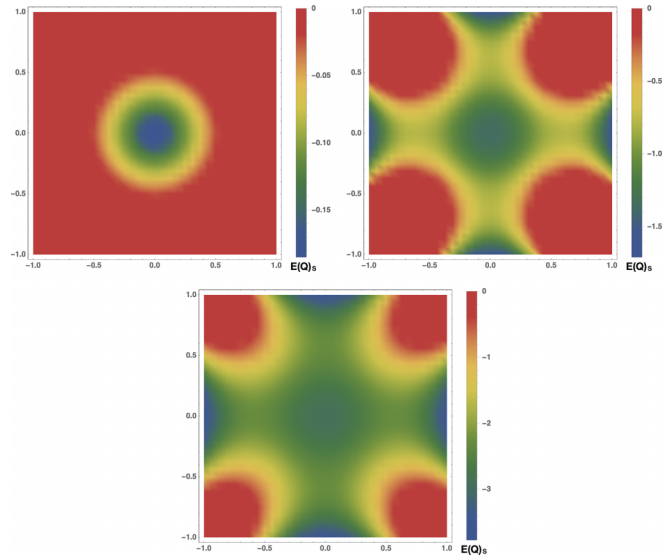

FIG. 6. Plots of the free energy $E(\mathbf{Q})_S$ of the superconducting state as a function of center-of-mass momentum $\mathbf{Q}$ (units $\sqrt{\Lambda}$) across the PDW transition. Clockwise from top left: $\nu V_0 = 0.16/4\pi, 0.2/4\pi, 0.24/4\pi$. The chemical potential is set to $\mu = 1$.

where $\bar{\xi}_{\mathbf{k}}(\mathbf{Q}) \equiv \xi_{\mathbf{k}+\frac{\mathbf{Q}}{2}} + \xi_{-\mathbf{k}+\frac{\mathbf{Q}}{2}}$, $E_{\mathbf{k}}(\mathbf{Q}) \equiv \sqrt{\bar{\xi}_{\mathbf{k}}(\mathbf{Q})^2 + 4\Delta_{\mathbf{k}}(\mathbf{Q})^2}$, and $\Delta_{\mathbf{k}}(\mathbf{Q}) = f_{\mathbf{k}}(\mathbf{Q})\bar{\Delta}(\mathbf{Q})$. Here $\bar{\Delta}(\mathbf{Q})$ is a quantity independent of the relative momentum and is determined self-consistently using the formula

$$1 = V_0 \sum_{\mathbf{k}} \frac{f_{\mathbf{k}}(\mathbf{Q})^2}{\sqrt{\bar{\xi}_{\mathbf{k}}(\mathbf{Q})^2 + 4 f_{\mathbf{k}}(\mathbf{Q})^2 \bar{\Delta}(\mathbf{Q})^2}}. \tag{G4}$$

The quantity $2\Delta_{\mathbf{k}}(\mathbf{Q})$ can be interpreted as the order parameter and takes the meaning of a superconducting gap while $E_{\mathbf{k}}(\mathbf{Q})$ is the quasiparticle energy. Plots of the $\mathbf{Q}$ dependent free energy and superconducting gaps $[\bar{\Delta}(\mathbf{Q})]$ in the continuum limit appear in Fig. 5 for $n = 1$ and $\mu = 1$ with $\nu V_0 = 4/4\pi$. For isotropic interactions, the function $\bar{\Delta}(\mathbf{Q})$ falls to zero for large $\mathbf{Q}$ uniformly in all directions; the free energy gain similarly approaches zero uniformly for large enough $\mathbf{Q}$ and the minimum occurs at $\mathbf{Q} = 0$. This signals a homogeneous pairing state. However, for anisotropic interactions, the gap function increases along the antinodal directions $[(Q_x, Q_y) = (\pm 1, 0), (0, \pm 1)]$. Correspondingly, the free energy gain is maximized along these directions indicating instability of the zero-$\mathbf{Q}$ phase towards a nonhomogeneous solution. In the presence of a lattice, we can similarly show that the gap (free energy gain) is bounded with a maximum (minimum) occurring at $\mathbf{Q} \neq 0, \mathbf{G}$ when both $n = 1, 2$ harmonics are included, signaling a PDW state. These conclusions are similar to two-body results discussed in Fig. 1. In an analogous manner, we also plot the evolution of the free energy as a function of V_0 for anisotropic interactions in Fig. 6. For weak enough interaction strength, we find that the free energy minimum occurs at $\mathbf{Q} = 0$. The minimum then shifts away from the homogeneous solution upon tuning the interaction strength to larger values consistent with the two-body solution in Fig. 3.

APPENDIX H: MANY-BODY FREE ENERGY AND NONHOMOGENEOUS GAP USING VARIATIONAL ANSATZ

Here we provide details leading to the expressions for the variational free energy and nonhomogeneous gap functions Eqs. (G3), (G4). To derive these equations, we take the expectation value of the total Hamiltonian Eq. (G2) with respect to the ground-state ansatz $|\Psi_{\mathrm{PDW}}\rangle$ Eq. (G2). The kinetic energy term yields

$$\langle \Psi_{\mathrm{PDW}} | \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} | \Psi_{\mathrm{PDW}} \rangle = \sum_{\mathbf{k}} (\xi_{\mathbf{k}+\mathbf{Q}/2} + \xi_{-\mathbf{k}+\mathbf{Q}/2}) v_{\mathbf{k}}(\mathbf{Q})^2, \tag{H1}$$

where the two terms on the right-hand side with relative momenta $\mathbf{Q}$ correspond to the two spin projections $(\uparrow, \downarrow)$, respectively. Similarly the interaction term yields

$$\langle \Psi_{\mathrm{PDW}} | \sum_{\mathbf{k}\mathbf{k}'\mathbf{Q}} V_{\mathbf{k}\mathbf{k}'}(\mathbf{Q}) c^{\dagger}_{\mathbf{k}+\mathbf{Q}/2\uparrow} c^{\dagger}_{-\mathbf{k}+\mathbf{Q}/2\downarrow} c_{-\mathbf{k}'+\mathbf{Q}/2\downarrow} c_{\mathbf{k}'+\mathbf{Q}/2\uparrow} | \Psi_{\mathrm{PDW}} \rangle = \sum_{\mathbf{k},\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}(\mathbf{Q}) u_{\mathbf{k}}(\mathbf{Q}) v_{\mathbf{k}}(\mathbf{Q}) u_{\mathbf{k}'}(\mathbf{Q}) v_{\mathbf{k}'}(\mathbf{Q}). \tag{H2}$$

The wave function components $u_{\mathbf{k}}(\mathbf{Q}), v_{\mathbf{k}}(\mathbf{Q})$ satisfy the constraint $u_{\mathbf{k}}(\mathbf{Q})^2 + v_{\mathbf{k}}(\mathbf{Q})^2 = 1$ and can be parameterized as $u_{\mathbf{k}}(\mathbf{Q}) = \sin\theta_{\mathbf{k},\mathbf{Q}}$ and $v_{\mathbf{k}}(\mathbf{Q}) = \cos\theta_{\mathbf{k},\mathbf{Q}}$. We now minimize the total expectation value $E(\mathbf{Q})_S = \langle \Psi_{\mathrm{PDW}} | \mathscr{H} | \Psi_{\mathrm{PDW}} \rangle$ with

respect to the parameter $\theta_{\mathbf{k},\mathbf{Q}}$ and we obtain the condition

$$\tan 2\theta_{\mathbf{k},\mathbf{Q}} = \frac{-2\Delta_{\mathbf{k}}(\mathbf{Q})}{\left(\xi_{\mathbf{k}+\mathbf{Q}/2} + \xi_{-\mathbf{k}+\mathbf{Q}/2}\right)} \equiv \frac{-2\Delta_{\mathbf{k}}(\mathbf{Q})}{\bar{\xi}_{\mathbf{k}}(\mathbf{Q})}, \tag{H3}$$

so that $2u_{\mathbf{k}}(\mathbf{Q})v_{\mathbf{k}}(\mathbf{Q}) = \sin 2\theta_{\mathbf{k},\mathbf{Q}} = \frac{2\Delta_{\mathbf{k}}(\mathbf{Q})}{E_{\mathbf{k}}(\mathbf{Q})}$ and $v_{\mathbf{k}}(\mathbf{Q})^2 - u_{\mathbf{k}}(\mathbf{Q})^2 = \cos 2\theta_{\mathbf{k},\mathbf{Q}} = -\frac{\bar{\xi}_{\mathbf{k}}(\mathbf{Q})}{E_{\mathbf{k}}(\mathbf{Q})}$. As stated in the main text, here we have defined the quantities

$$\Delta_{\mathbf{k}}(\mathbf{Q}) \equiv -\frac{1}{2}\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}(\mathbf{Q}) \sin 2\theta_{\mathbf{k},\mathbf{Q}} \tag{H4}$$

$$= -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}(\mathbf{Q}) u_{\mathbf{k}'}(\mathbf{Q}) v_{\mathbf{k}'}(\mathbf{Q}) \tag{H5}$$

$$E_{\mathbf{k}}(\mathbf{Q}) \equiv \sqrt{\bar{\xi}_{\mathbf{k}}(\mathbf{Q})^2 + 4\Delta_{\mathbf{k}}(\mathbf{Q})^2}. \tag{H6}$$

Using these definitions and the normalization relation $u_{\mathbf{k}}(\mathbf{Q})^2 + v_{\mathbf{k}}(\mathbf{Q})^2 = 1$, we can obtain explicit expressions for the variational parameters $u_{\mathbf{k}}(\mathbf{Q})$, $v_{\mathbf{k}}(\mathbf{Q})$ as

$$v_{\mathbf{k}}(\mathbf{Q}) = \sqrt{\frac{1}{2}\left(1 - \frac{\bar{\xi}_{\mathbf{k}}(\mathbf{Q})}{E_{\mathbf{k}}(\mathbf{Q})}\right)}$$

$$u_{\mathbf{k}}(\mathbf{Q}) = \sqrt{\frac{1}{2}\left(1 + \frac{\bar{\xi}_{\mathbf{k}}(\mathbf{Q})}{E_{\mathbf{k}}(\mathbf{Q})}\right)}. \tag{H7}$$

To arrive at the condition for the nonuniform gap function [Eq. (G4) main text], we substitute the variational parameters into the definition for $\Delta_{\mathbf{k}}(\mathbf{Q})$ above. After further utilizing the form of the interaction in Eq. (1) we obtain the gap equation

$$\Delta_{\mathbf{k}}(\mathbf{Q}) = \frac{V_0}{2}\sum_{\mathbf{k}'} \frac{2\Delta_{\mathbf{k}'}(\mathbf{Q})}{E_{\mathbf{k}'}(\mathbf{Q})} f_{\mathbf{k}}(\mathbf{Q}) f_{\mathbf{k}'}(\mathbf{Q}). \tag{H8}$$

The ansatz that solves the above equation takes the form $\Delta_{\mathbf{k}}(\mathbf{Q}) = f_{\mathbf{k}}(\mathbf{Q})\bar{\Delta}(\mathbf{Q})$ where $\bar{\Delta}(\mathbf{Q})$ is independent of the relative momentum $\mathbf{k}$. Substituting the ansatz into $\Delta_{\mathbf{k}}(\mathbf{Q})$, the gap equation simplifies to Eq. (G4)

$$1 = V_0 \sum_{\mathbf{k}} \frac{f_{\mathbf{k}}(\mathbf{Q})^2}{\sqrt{\bar{\xi}_{\mathbf{k}}(\mathbf{Q})^2 + 4 f_{\mathbf{k}}(\mathbf{Q})^2 \bar{\Delta}(\mathbf{Q})^2}}. \tag{H9}$$

We can further easily obtain the superconducting contribution to the free energy by utilizing Eqs. (G4), (H1), (H2), and (H7). Substituting Eq. (H7) into Eqs. (H1), (H2) and utilizing Eq. (G4), we obtain

$$E(\mathbf{Q})_S = \langle \Psi_{\mathrm{PDW}} | \mathscr{H} | \Psi_{\mathrm{PDW}} \rangle$$

$$= \frac{1}{2}\sum_{\mathbf{k}} \bar{\xi}_{\mathbf{k}}(\mathbf{Q}) \left[1 - \frac{\bar{\xi}_{\mathbf{k}}(\mathbf{Q})}{E_{\mathbf{k}}(\mathbf{Q})}\right] - \frac{4\bar{\Delta}(\mathbf{Q})^2}{V_0}, \tag{H10}$$

which is Eq. (G3) above.

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