Phonon-Mediated Superconductivity in Doped Monolayer Materials

Even Thingstad, Akashdeep Kamra, Justin W. Wells, and Asle Sudbø
Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

Insight into why superconductivity in pristine and doped monolayer graphene seems strongly suppressed has been central for the recent years’ various creative approaches to realize superconductivity in graphene and graphene-like systems. We provide further insight by studying electron-phonon coupling and superconductivity in doped monolayer graphene and hexagonal boron nitride based on intrinsic phonon modes. Solving the graphene gap equation using a detailed model for the effective attraction based on electron tight binding and phonon force constant models, the various system parameters can be tuned at will. Our results show that the Coulomb interaction plays a major role in suppressing superconductivity at realistic dopings and induces slight gap modulations along the Fermi surface. Motivated by the direct onset of a large density of states at the Fermi surface for small charge dopings in hexagonal boron nitride, we also calculate the dimensionless electron-phonon coupling strength there. Somewhat counter-intuitively, however, the comparatively large density of states cannot immediately be capitalized on, and the charge doping necessary to obtain significant electron-phonon coupling is similar to the value in graphene.

I. INTRODUCTION

The discovery of graphene has attracted massive attention in condensed matter physics, stimulating an enormous number of theoretical and experimental investigations into a class of novel materials broadly denoted as Dirac materials [1-5]. Among their interesting properties is the Dirac-cone shaped electron band structure at half filling, enabling the study of relativistic physics in a condensed matter setting [5-8]. However, the cone structure with a vanishing density of states and Fermi-surface at the Dirac point suppresses phenomena such as superconductivity, which precisely rely on the existence of a Fermi-surface.

In spite of this obstacle, there is a plethora of graphene-like systems where superconductivity has been predicted or observed. In carbon nanotubes and the carbon based fullerene crystals also known as “buckyballs”, superconductivity was observed already decades ago in crystals intercalated with potassium [9-11]. Superconductivity is also well known in graphite intercalation compounds [12-16], where the interlayer interactions and the additional dopant phonon modes enhance superconductivity [13]. A similar picture arises also for intercalated bilayer graphene, where interlayer interactions have been predicted to be crucial for the resulting superconductivity [17]. In bilayer graphene, a different route to superconductivity is the magic angle twist approach [18-21], which has been shown to boost phonon mediated superconductivity significantly. In addition to these phonon-based mechanisms, superconductivity may also be induced by proximity [22,25]. The resulting superconductivity in graphene will necessarily inherit extrinsic key properties from the superconductor it is placed in proximity to [26].

Although superconductivity is already well established in a multitude of these graphene-like systems, its observation in monolayer graphene has proven very challenging. The key issue is to boost the dimensionless electron-phonon coupling (EPC) strength $\lambda$. This quantity is determined by both the density of states at the Fermi level and the strength of the effective phonon-mediated potential. The first challenge that has to be overcome is therefore doping the system away from the Dirac point. The primary ways of doing this are chemical doping [27,31] and deposition of elements onto (or under) the graphene sheet [32-41]. Using these methods, doping of order $\pm 1$ eV has been achieved [30]. Second, one must make sure that $\lambda$ has a sufficiently large value at the achievable doping. It has been suggested that applying a mechanical strain may enhance the electron-phonon coupling strength [39]. More importantly, however, the additional dopant phonon modes in decorated monolayer graphene enhance the electron-phonon coupling strength [39,41]. In these systems, one has even observed evidence [41] for the desired monolayer graphene superconductivity with a critical temperature of about 6 K. A similar mechanism is responsible for the superconducting transition which has been observed [42] through transport measurements in the weakly coupled layers of graphene laminates.

Regardless of doping, however, the EPC strength $\lambda$ can be measured by examining kinks and broadening in the electronic band structure using angular resolved photo-emission spectroscopy (ARPES) [43-45]. At realistic doping energies in the vicinity of the van Hove singularity in the $\pi$-band, $\lambda$-values of 0.2 to 0.3 have been predicted and measured experimentally [45-47]. This is of the same order as in many known conventional superconductors [48]. In light of this, superconductivity in single-layer graphene with reasonable critical temperatures does not seem inconceivable even without applied mechanical strain or additional dopant phonon modes. This does not seem to be borne out. As mentioned in the previous paragraph, quite elaborate schemes seem to be required in order to get measurable superconducting critical temperatures in graphene. Why is this? Are there additional fundamental obstacles beyond the difficulty of achieving adequate doping levels?
The Coulomb interaction \( \lambda \) could be such an obstacle. In normal superconducting materials, it does not play a significant role in reducing \( T_c \), since the effective phonon-mediated potential is attractive only in a small region around the Fermi surface, whereas the repulsive Coulomb interaction has much longer Brillouin zone variations. The mechanism at work, retardation, can be seen by solving the gap equation with a simplified model \[50\] for the combined potential. Due to the modest electron-phonon coupling strength in graphene, however, we do expect significant effects of Coulomb interactions \[39 \] \[49 \] \[51\]. A crude estimate of the Anderson-Morel renormalization of the dimensionless EPC strength \( \lambda \) shows that the renormalization is of the same order as \( \lambda \) itself.

In this paper, we therefore perform detailed calculations of the electron-phonon coupling strength based on an electron tight binding model and a phonon force constant model. We then solve the gap equation both in the presence and absence of a Hubbard-type Coulomb interaction. Whereas many works have looked into the electron phonon coupling strength and made predictions about the superconducting pairing and critical temperature based on this \[58 \] \[40 \] \[22 \] \[54\], we are not aware of works using a detailed model such as ours for the phonon-mediated and Coulomb interaction to actually solve the gap equation and determine the Brillouin zone gap structure. The ability to tune the various parameters in this model opens up for an investigation of how the various physical mechanisms affect superconducting transition temperature and superconducting properties, and the understanding of why this is essential in the pursuit of realizing superconductivity in monolayer graphene, based on the intrinsic in-plane phonon modes.

Our results show that, whereas reasonable critical temperatures are possible in graphene in the absence of Coulomb interaction, its inclusion significantly suppresses the critical temperature even for relatively small Coulomb interactions. Furthermore, and in spite of the anisotropic Fermi surface at significant doping, the gap is shown to be surprisingly uniform along the Fermi surface in the absence of Coulomb interaction, but its inclusion induces slight gap modulations along the Fermi surface. While estimates for the critical temperature are notoriously unreliable due to the exponential sensitivity on \( \lambda \) and its renormalization, the gap non-uniformity is a lot more stable, and could in principle be measured with ARPES. We also look into the contributions to the electron-phonon coupling from the various phonon modes in the system and identify the high-energy phonons as the most significant for the superconducting instability in the realistically achievable doping regime, consistent with previous results \[39\].

The two-dimensional material hexagonal boron nitride (h-BN) was discovered \[2\] shortly after graphene \[1\] using the same micromechanical cleavage technique to exfoliate monolayers from the stacks of weakly interacting layers also known as van der Waals materials. In many respects, the two are very similar \[51\]. They have the same lattice structure and a similar lattice constant, which makes h-BN a good substrate for graphene \[55 \] \[56 \] and suitable for graphene heterostructure engineering \[57\]. Like graphene, it also has strong chemical bonding, and a comparable phonon Debye frequency \[58\]. Unlike graphene, however, boron nitride has two different ions, boron and nitrogen, on the two honeycomb sublattices. This has dramatic consequences for the electronic band structure, since the Dirac cone in graphene is protected by time reversal and inversion symmetry. Breaking of the latter symmetry therefore renders hexagonal boron nitride a large gap insulator \[59\].

The possibility of superconductivity in doped hexagonal boron nitride is a lot less studied than in doped graphene, but a recent density functional theory study \[60\] suggests that decorated h-BN may become superconducting with a transition temperature of up to 25 K. Although the dopant phonon modes are again responsible for this relatively large transition temperature, this also hints at possibilities for superconductivity mediated by intrinsic in-plane phonon modes. Furthermore, and very different from graphene, the parabolic nature of the electron band close to the valence band maximum gives a direct onset of a large density of states even at small charge doping. Motivated by this, we use the same methodology as in the graphene case to calculate the dimensionless electron-phonon coupling strength \( \lambda \) for hexagonal boron nitride. Somewhat counter-intuitively, however, our results show that the electron-phonon coupling strength at very small charge doping is smaller for boron nitride than for graphene precisely because of this large density of states. At somewhat larger charge doping, the electron-phonon coupling strengths are similar.

In Section \( \text{II} \) of this paper, we first present the free electron and the free phonon models for graphene briefly, followed by a more thorough derivation of the tight binding electron-phonon coupling. In Section \( \text{III} \) we find quasimomentum expressions for the Coulomb interaction based on a real-space density-density Coulomb interaction lattice model. In Section \( \text{IV} \) we introduce the assumed pairing, resulting gap equation and effective phonon-mediated potential, before presenting the numerical results for graphene in Section \( \text{V} \). In Section \( \text{VI} \) we discuss some qualitative aspects of these results. Switching to boron nitride in Section \( \text{VII} \) we discuss how the opening of a gap changes the band structure and phonon coupling. Finally, the paper is summarized in Section \( \text{VIII} \).

\section*{II. ELECTRONS, PHONONS, AND ELECTRON-PHONON COUPLING}

We consider a model for electrons on the graphene lattice, and allow for lattice site vibrations. For the electrons, we use a nearest neighbour tight binding model \[4\] describing the \( \pi \)-bands, as explained in further detail in
The phonon mode frequencies are denoted by the plane phonon Hamiltonian (see Appendix B for details).

The electron-phonon coupling model is derived by assuming the electrons to follow the lattice site ions adiabatically, and by Taylor expanding the overlap integral \( t_{ij} \) in the hopping Hamiltonian

\[
H = - \sum_{(i,j)} (t_{ij} c_i^\dagger c_j + \text{h.c.})
\]  

(1)

to linear order in the deviations. Considering only the nearest neighbour hoppings, we obtain

\[
t_{i+\delta_A,i} = t_1 + (u_{i+\delta_A} - u_i) \cdot \nabla t_1(\delta),
\]  

(2)

where \( t_1 \) is the nearest neighbour hopping amplitude, \( u_i \) is the ionic displacement of lattice site \( i \) from its equilibrium position, and the overlap integral \( t_1(\delta) \) is regarded as a function of the relative position \( \delta \) of the two lattice sites \( i \) and \( i + \delta_A \), where \( \delta_A \) is the equilibrium nearest neighbour vector from the A to the B sublattice. Due to the mirror-symmetry about the line connecting the lattice sites \( i \) and \( i + \delta_A \), the electron-phonon coupling can be written as

\[
H_{\text{el-ph}} = \frac{\gamma}{d^2} \sum_{i \in A, \delta_A} \delta_A \cdot (u_{i+\delta_A} - u_i) (e_i^\dagger e_{i+\delta_A}^\dagger + \text{h.c.}),
\]  

(3)

where \( \gamma = -d \log t_1/d \log d \) is a dimensionless number of order 1, and \( d \) is the equilibrium nearest neighbour distance, which we use as our unit of length. In quasimomentum-space, this gives the electron-phonon coupling

\[
H_{\text{el-ph}} = \sum_{k,q} \sum_{\eta} g_{\eta q}^\eta e_{\eta q}^\dagger e_{\eta q} + (a_{\eta q}^\dagger a_{\eta q}) c_{k+q,\eta}^\dagger c_{k,\eta},
\]  

(4)

where \( \eta, \eta' = \pm \) denote electron bands and \( \nu \in \{0, 1, 2, 3\} \) labels in-plane phonons. To linear order in the lattice site deviations, the out-of-plane phonon modes do not couple to the electrons due to the assumed \( z \rightarrow -z \) mirror symmetry of the system. The coupling \( g_{\eta q}^\eta \) is given by

\[
g_{\eta q}^\eta = \frac{g_0}{\sqrt{N_A}} \sqrt{\frac{\omega_D}{\omega_{\nu q}^\text{ph}}} \sum_{\delta_A} \left( \frac{\delta_A}{d} \right) \left[ e^{iq\delta_A} e_{\nu q}^\dagger (q) - e_{\nu q}^\dagger (q) \right] \left[ e^{ik\delta_A} F_{A\eta}^\star (k + q) F_{B\eta} (k) + e^{-i(k+q)\delta_A} F_{B\eta}^\star (k + q) F_{A\eta} (k) \right],
\]  

(5)

where \( F_{D\eta}(k) \) is the sublattice amplitude of electron band \( \eta \) at quasimomentum \( k \) and follows from the diagonalization of the free electron model, as elaborated in Appendix A. Similarly, \( e_{\nu q}^\dagger (q) \) is the phonon polarization vector at sublattice \( D \in \{A, B\} \) for the phonon mode \( (q, \nu) \), and follows from diagonalization of the in-plane phonon Hamiltonian (see Appendix B for details). The phonon mode frequencies are denoted by \( \omega_{\nu q}^\text{ph} \). \( N_A \) is the number of lattice sites on the A sublattice, and the constant \( g_0 \) is given by

\[
g_0 = \sqrt{\frac{\hbar^2}{2 M d^2}} \frac{1}{\hbar \omega_{\nu q}^\Gamma} f_\gamma,
\]  

(6)

where \( M \) is the carbon atom mass, and \( \omega_{\nu q}^\Gamma \) is a phonon energy scale given by the optical phonon frequency at the \( \Gamma \)-point \( q = (0,0) \).

To quantify the strength of the electron-phonon coupling, one may introduce the dimensionless electron-phonon coupling strength parameter \[ 44, 64 \]

\[
\lambda_k = \sum_{q, \nu} \frac{2}{\hbar \omega_{\nu q}^\text{ph}} \left| g_{k,\nu q} \right|^2 \delta(\epsilon_{-k+q} - \epsilon_{-k} - \hbar \omega_{\nu q}),
\]  

(7)

which can be interpreted as a sum over all phonon-assisted decay processes and is directly related to the lifetime of the state \((-k, k)\). Usually, the definition of \( \lambda_k \) also includes decay processes to other electron bands, but since the energy change of an electron in a decay process is limited by the comparatively small phonon Debye frequency \( \omega_D \) and the \( \pi \)-band only overlaps with the lower lying \( \sigma \)-bands at unrealistic doping levels \[ 55, 65 \], these processes are not relevant for us.

Averaging \( \lambda_k \) over the Fermi surface corresponding to the energy of the incoming momentum often provides a simple and useful tool for understanding the dependence of the critical temperature of a superconductor on other system parameters through the BCS formula

\[
k_B T_c \approx \hbar \omega_D \exp(-1/\lambda),
\]  

where \( \lambda = \langle \lambda_k \rangle_{FS} \).

### III. COULOMB INTERACTION

To include the effect of the Coulomb interaction, we use the effective lattice model.
where \( n \) labels the contribution from the interaction between \( n \)-th nearest neighbours, \( u_{ij} \equiv u_n \) when \( i \) and \( j \) are \( n \)-th nearest neighbours, \( \eta_i \) are band indices, \( \sigma \) and \( \sigma' \) are spin indices, and the scattering amplitudes \( E_{\eta_1 \cdots \eta_4}^{\sigma \sigma',n} \) are derived in Appendix [D]. Since we are interested in single-pairing superconductivity at \( \pm \mathbf{k} \), as discussed further in section [IV], and are interested in the pairing potential close to the Fermi surface for the system doped away from the Dirac point, we consider only one band, letting \( \eta_1 = \eta_2 = \eta_3 = \eta_4 \equiv \eta_1 \), and opposite spin scatterings with \( \sigma \neq \sigma' \). The Coulomb interaction potential relevant for spin-singlet electron-pairing is therefore

\[
V^C = \sum_n \frac{u_n}{N_A} \sum_{\mathbf{k} \mathbf{k}'} \sum_{\eta_1 \eta_2 \eta_3 \eta_4} E_{\eta_1 \eta_2 \eta_3 \eta_4}^{\sigma \sigma',n} (\mathbf{k}, \mathbf{k}', \mathbf{q}) c_{\eta_1 \sigma}(\mathbf{k} + \mathbf{q}) c_{\eta_1 \sigma}^\dagger(\mathbf{k} - \mathbf{q}) c_{\eta_3 \sigma'}(\mathbf{k}) \tag{9}
\]

for the \( n \)-th nearest neighbour contribution. This quantity is the Coulomb contribution to the effective potential involved in the gap equation in section [IV].

The effective potential has to be calculated separately for the three cases of on-site, inter-sublattice and intra-sublattice interaction, and the precise expressions are given in Appendix [D].

### IV. PAIRING AND GAP EQUATION

The in-plane phonons yield an effective interaction between the electrons in the system that may cause pairing and superconductivity. Assuming spin-singlet pairing at \( \pm \mathbf{k} \) and considering only the electron band \( \pi^- \), the relevant interaction can be written in the form

\[
V = \sum_{\mathbf{k} \mathbf{k}'} V_{\mathbf{k} \mathbf{k}'} c_{\pi^-}(\mathbf{k}') c_{\pi^-}(\mathbf{k}) \tag{12}
\]

with a potential \( V_{\mathbf{k} \mathbf{k}'} \) that contains contributions both from the Coulomb potential and an effective phonon-mediated potential \( V_{\mathbf{k} \mathbf{k}'}^{\text{ph-m.}} \), so that

\[
V_{\mathbf{k} \mathbf{k}'} = V_{\mathbf{k} \mathbf{k}'}^C + V_{\mathbf{k} \mathbf{k}'}^{\text{ph-m.}} \tag{13}
\]

The Coulomb contribution is given by the expressions discussed in section [III] whereas the effective phonon-mediated potential follows from a diagrammatic expansion [66], or by using an appropriate canonical transformation [67]. To lowest order, it is given by

\[
V_{\mathbf{k} \mathbf{k}'}^{\text{ph-m.}} = \sum_{\nu} \frac{\hbar \omega_{\mathbf{k} \mathbf{k}'}}{(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k} + \mathbf{q}})^2 + (\hbar \omega_{\mathbf{q}})^2} \tag{14}
\]

where the quasimomentum \( \mathbf{q} \) is fixed by \( \mathbf{k}' = \mathbf{k} + \mathbf{q} \).

Due to the singlet pairing assumption, the gap has to be symmetric under \( \mathbf{k} \to -\mathbf{k} \) and therefore, the potential \( V_{\mathbf{k} \mathbf{k}'} \) can be replaced with the symmetrized potential

\[
V_{\mathbf{k} \mathbf{k}'}^{\text{symm}} = \frac{1}{2} (V_{\mathbf{k} \mathbf{k}'} + V_{\mathbf{k} \mathbf{k}}) \tag{15}
\]

which is symmetric under \( \mathbf{k} \to -\mathbf{k} \) and \( \mathbf{k}' \to -\mathbf{k}' \), as well as interchange of the incoming and outgoing momenta \( \mathbf{k} \) and \( \mathbf{k}' \).

To proceed, we have to solve the gap equation

\[
\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k} \mathbf{k}'}^{\text{symm}} \chi_{\mathbf{k}' \mathbf{k}} \Delta_{\mathbf{k}'} \tag{16}
\]

with susceptibility

\[
\chi_{\mathbf{k}} = \frac{\tanh \beta E_{\mathbf{k}} / 2}{2E_{\mathbf{k}}} \quad E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2} \tag{17}
\]

where \( E_{\mathbf{k}} \) is the quasiparticle excitation energy, and \( \xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu \) is the single particle energy \( \epsilon_{\mathbf{k}} \) measured relative to the Fermi surface at chemical potential \( \mu \).

In the special case \((T_c - T)/T_c \ll 1\), i.e. just below the critical temperature, the gap is small, and the selfconsistent equation may be linearized in the gap.
gives an eigenvalue problem linear in the eigenvectors and non-linear in the eigenvalue. We determine the critical temperature and the structure of the gap $\Delta_k$ exactly at the superconducting instability by solving this eigenvalue problem numerically. Further details are given in Appendix $E$.

V. GRAPHENE NUMERICAL RESULTS

A. Parameter values and free spectra

We set the equilibrium electron hopping amplitude $t_1$ to 2.8 eV [49]. The resulting electron band structure for the $\pi$-bands of graphene is shown in Fig. 1(a). For the phonon force constant model used to derive the phonon spectrum, we use the same parameter values as Ref. [61], and the resulting excitation spectrum is shown in Fig. 1(b).

We fix the dimensionless constant $\gamma$ to given reasonable values [46] for the dimensionless electron-phonon coupling strength $\lambda$. With phonon energy scale $\hbar\omega_T = 0.20$ eV and nearest neighbour distance $d = 1.42$ Å [68], this gives $g_0 = 0.29$ eV. All system parameters involved in the calculation of the energy scale are tabulated in Appendix $F$.

In the Coulomb interaction, we include on-site up to and including third-nearest neighbour interactions. Based on random phase approximation (RPA) calculations of these parameters in Ref. [51], we fix the ratio of the interaction parameters $u_n$, and use the on-site interaction strength $u_0$ to tune all the interaction parameters we include to investigate the effect of Coulomb interaction.

B. Electron-phonon coupling and effective potential

Using the parameter values in the preceding subsection, one may calculate the electron-phonon coupling strength $\lambda$ as function of the chemical potential $\mu$. This is shown in Fig. 2 with contributions from the four in-plane phonon modes shown in color. The parameter $\lambda$ incorporates both the strength of the effective potential at the Fermi surface and the density of states. Since the latter has a very systematic variation with the chemical potential, $\lambda$ and the electronic density of states have similar profiles, as also shown in Fig. 2. In the low doping regime, the optical phonon modes, and the highest energy mode in particular, dominate the electron-phonon coupling strength completely. Due to the phonon energy in a given scattering process, as shown in the inset, the linear increase in electron-phonon coupling strength with chemical potential starts an energy scale of 0.2 eV below $\mu = 0$, corresponding to the phonon Debye frequency. Similarly, the peak in $\lambda$ is shifted below the van Hove
FIG. 3. Graphene effective interaction $V_{\text{ph-m}}^{\text{ph-m}}$ in eV for incoming electron momentum $k$ (black dot) at outgoing momentum $k'$ indicated by the position in the plot.

FIG. 4. Decomposition of the effective interaction $V_{\text{ph-m}}^{\text{ph-m}}$ in eV for incoming momentum as in the upper right subfigure of Fig. 3 into contributions from the different in-plane phonon modes, where mode 0 has the lowest and mode 3 the highest energy. The high energy modes corresponding to large mode index or large quasimomentum scattering give the most significant contribution to the total effective potential.

FIG. 5. (a) Graphene Brillouin zone with Fermi surface (green and red) for large doping. The hexagonal first Brillouin zone is shown in blue, whereas the rhombus (black) contains an equivalent set of points. Assuming superconducting pairing at $\pm k$, the effective potential $V_{\text{ph-m}}^{\text{ph-m}}$ is the interaction amplitude for scattering of the particles from $\pm k$ to $\pm k'$. Since the Fermi surface consists of two disconnected sections, there can be intra-section (green arrow) and inter-section (red arrow) scattering processes. (b) An electron on the Fermi surface with incoming momentum indicated by the black dot can be scattered to points on the Fermi surface labelled by the angles $\theta_1$ and $\theta_2$. (c) Effective phonon-mediated potential for incoming momentum indicated by the black dot in (b) to outgoing momentum on the Fermi surface as given by the angles $\theta_1$ and $\theta_2$. Contributions from the various phonon modes are shown in color, with the total effective potential in black. The high energy phonon modes at large quasimomentum scattering or high mode index dominate the potential.

The effective potential $V_{kk'}^{\text{ph-m}}$ is shown in Fig. 5, where each subfigure shows the potential at a given incoming momentum $k$ at various outgoing momenta $k'$. For an incoming momentum $k$, the potential is attractive in a finite region around the Fermi surface corresponding to the energy of the incoming momentum, and becomes repulsive when the net kinetic energy transfer exceeds the phonon energy scale.

The potential has contributions from the four in-plane phonon modes, and these contributions are shown in Fig. 6 for one of the incoming momenta in Fig. 5. The size of the region with attractive interaction is determined by

singularity.
the energy of the relevant phonon mode. The optical high-energy phonon modes therefore give largest attractive Brillouin zone area. Comparing the effective potential contribution from the various in-plane phonon modes on the Fermi surface, as shown in Fig. 4, furthermore reveals that the high-energy phonon modes corresponding to high mode index or large quasimomentum scattering also give rise to a stronger attractive potential at the important Fermi surface than their low-energetic counterparts. In total, this means that the high-energy phonon modes give the most significant contribution to the effective potential, and that it is primarily the high-energy phonon modes that may cause the superconducting instability.

C. Solutions of the gap equation

To contain the divergences of the effective electronic potential, we introduce an energy cutoff $\Lambda = 5$ eV in the potential. Solving the linearized self-consistent equation [10], we obtain the Brillouin zone gap structure at the critical temperature $T_c$ for which the superconducting instability occurs. This is shown in Fig. 6 in the absence of Coulomb interaction, where the superconducting gap at a given point is given by the color of the dot at the given position in the Brillouin zone. Choosing the points for which we solve the gap equation, the regions around the Fermi surface are particularly important, and therefore, we have a much larger density of points there. The gap equation solution shows that the gap has a given sign within the attractive region of the Brillouin zone for incoming momenta at or close to the Fermi surface. Outside this region, the gap changes sign, and subsequently decays to zero far away from the Fermi surface. Considering the gap amplitude along the Fermi surface furthermore shows that, although the Fermi surface itself is anisotropic for the given doping, the gap is constant along the Fermi surface.

Turning on a finite Coulomb interaction, the gap equation solution is shown in Fig. 7. The gap amplitude becomes finite far away from the Fermi surface, as seen both in the Brillouin zone gap profile and in the gap profile perpendicular to the Fermi surface (orange). Furthermore, the Coulomb potential introduces modulations of the superconducting gap on the Fermi surface (green). A finite Coulomb interaction also decreases the critical temperature significantly, even for rather small interaction strengths. This is shown in Fig. 8 which shows the dependence of the critical temperature on the overall Coulomb interaction strength represented by the on-site interaction $u_0$. The data points from the solution of the gap equation have been fitted to the simple functional form that is expected from the Anderson-Morel model [50], as discussed in Appendix [6].

VI. DISCUSSION OF GRAPHENE RESULTS

One of the main results above is the dramatic decrease in critical temperature caused by moderate repulsive Coulomb interaction. In conventional superconductors, the effect of a Coulomb interaction is small, and the quantitative effect on the critical temperature can be incorporated through renormalization of the electron-phonon coupling strength $\lambda$ in the simple BCS result $k_B T_c = \hbar \omega_D \exp(-1/\lambda)$ according to $\lambda \rightarrow \lambda - \mu^*$, where

$$\mu^* = \frac{\hat{u}}{1 + \hat{u} \log(W/\hbar \omega_D)}.$$  (18)

Here, $\hat{u} = u N_0$, where $u$ is the constant repulsive interaction strength that is added on top of the attractive interaction close to the Fermi surface, and $N_0$ is the density of states at the Fermi surface, whereas $W$ is the band width and $\omega_D$ the Debye frequency. For strong Coulomb repulsion, the renormalization is suppressed down to values of $1/\log(W/\hbar \omega_D)$, so that Cooper pair formation is possible despite the Coulomb repulsion being much stronger than the attraction at the Fermi surface.

In the graphene case, simple estimates for the renormalization $\mu^*$ gives a value of 0.2 in the presence of strong Coulomb interaction. This is larger, but not very far away from first principle calculations [39] arriving at 0.10-0.15. This is of the same order as the electron-phonon coupling strength itself when we dope the system down towards the van Hove singularity. Since the simple Anderson-Morel model predicts absence of superconductivity for $\mu^* \geq \lambda$ and we expect to be quite close to this situation, based on these simple estimates, we would expect the Coulomb interactions to have a dramatic effect on the critical temperature of the superconducting transition. Our detailed solution of the gap equation in the presence of Coulomb interaction, confirms that the Coulomb interaction reduces the critical temperature significantly, even at rather small Coulomb interaction strengths. Furthermore, this implies that although boosting the electron-phonon coupling $\lambda$ would be essential for realizing superconductivity in graphene or graphene-like materials, within the realistic regime for $\lambda$, one cannot make predictions regarding superconductivity without also taking the repulsive Coulomb interaction into account explicitly.

Typically, calculations of the critical temperature are notoriously unreliable. On the other hand, the Fermi surface structure of the gap calculated in this paper should give reasonable estimates for the k-space modulation of the gap on the Fermi-surface. In the absence of a Coulomb interaction, the gap is remarkably uniform on the Fermi surface, the highly anisotropic shape of the Fermi surface itself notwithstanding. It is the Coulomb interaction that introduces non-uniform gap structure along the Fermi surface. This is in accordance with the observation that systems with strong Coulomb interaction tend to have anisotropic gap structures [20]. Such gap structures can in principle be measured by ARPES.
FIG. 6. Superconducting gap structure in the absence of Coulomb interaction at critical temperature $T_c$ and the indicated chemical potential $\mu$. (a) shows the hexagonal Brillouin zone of the triangular Bravais lattice in magenta. The rhombus contains an equivalent set of quasimomenta. Since the gap is symmetric under $k \rightarrow -k$, we may consider only half of this rhombus. The green contours indicate the Fermi surface, and the short orange line is perpendicular to the Fermi surface. (b) shows the gap structure around the point $K'$ in color for the given interaction parameters $u_n$. The insets show the gap structure perpendicular to (orange) and along (green) the Fermi surface.

FIG. 7. Superconducting gap structure at non-zero repulsive Coulomb interaction. See Fig. 6 for a detailed figure description. At finite repulsive interaction, the gap remains finite far away from the Fermi surface, as seen both in the triangle plot and the plot of the gap structure perpendicular to the Fermi surface. The Coulomb interaction also introduces slight gap modulations along the Fermi surface.

In our calculations, we have based our parameter choices on known values for graphene when the Fermi surface coincides with the Dirac point. As shown in Fig. 2, realizing values for $\lambda$ approaching 0.2 or 0.3 requires significant doping levels approaching the limits of realistically achievable doping. Doping is well known to affect the Coulombic screening length, and we would also expect the details of the phonon modes and the interaction parameters to change. We furthermore expect these changes to depend on the method chosen to dope graphene [40]. To understand why realizing superconductivity in graphene is so challenging, it is nevertheless
The atoms on the two different sublattices are boron and nitrogen. The associated sublattice symmetry breaking opens a gap in the electronic spectrum, and in this section, we discuss how this affects the electron-phonon coupling.

Due to the sublattice symmetry breaking of boron nitride, the electron tight binding model in Eq. (1) has to be modified by the addition of a sublattice asymmetric potential term

$$H_{\text{hm}} = \frac{\Delta_{\text{BN}}}{2} \left( \sum_{iA} c_i^\dagger c_i - \sum_{jB} c_j^\dagger c_j \right).$$

(19)

The resulting electron band structure is shown in Fig. (2a), where $t_1 = 2.92 \text{ eV}$ and $\Delta_{\text{BN}} = 4.3 \text{ eV}$.

For the phonon excitation spectrum, we again use a force constant model as outlined in Appendix B. Values for the boron nitride force constants are obtained by fitting the excitation energies at the high symmetry points to values from density functional theory values in Ref. 58 as discussed in Appendix C. The resulting excitation spectrum is shown in Fig. (2b).

As in the graphene calculation, the electron-phonon coupling is obtained by Taylor-expanding the hopping element integral in Eq. (1). The resulting electron-phonon coupling matrix element is similar, but due to the rescaling of the deviation discussed in Appendix C, the expression for the electron-phonon coupling matrix element $\tilde{g}^{\nu\nu'}_{kk'}$ in Eq. (5) is modified according to $c_{\nu}^{D}(\mathbf{q}) \rightarrow c_{\nu}^{D}(\mathbf{q})/\sqrt{\mu_D}$. Here, $\nu_D$ relates the sublattice mass $M_D$ and the effective mass $\tilde{M} = \sqrt{M_A M_B}$ through $M_D = \mu_D \tilde{M}$. To compare the boron nitride results with graphene, we set the value of the dimensionless quantity $\gamma$ to the same value that was used for graphene. All quantities involved in the calculation of the electron-phonon coupling energy scale $g_0$ are listed in Appendix F.

Averaging the dimensionless electron-phonon coupling strength $\lambda_k$ over the Fermi surface at chemical potential $\mu$ gives the result shown in Fig. (10). The inset shows the same electron-phonon coupling $\lambda$ as function of the charge doping $n$ corresponding to each chemical potential $\mu$ for both boron nitride and graphene.

Unlike the graphene electron-phonon coupling strength shown in Fig. (2), the electron-phonon coupling strength of boron nitride is qualitatively different from the electronic density of states. At the valence band edge, the electron density of states has a discontinuous jump, but $\lambda$ remains negligible within 0.15 eV of the band edge, and subsequently increases roughly linearly. Due to the direct onset of a large density of states in boron nitride, it is tempting to assert that even small charge dopings could quickly give rise to appreciable electron-phonon coupling strengths. This is not the case. The electron-phonon coupling matrix element $|g^{\nu\nu'}_{kk'}|^2$ in Eq. (5) also plays an essential role for the overall value of the electron-phonon coupling strength, and is suppressed when the Fermi surface is small. In fact, the comparison between

![Graphene-like materials. In particular, we consider hexagonal boron nitride (h-BN), which is a two-dimensional material very similar to graphene, but where useful to understand how superconductivity would work if these parameters remained unchanged by the doping.

In practice, graphene is often mounted on a substrate. A small substrate coupling can be included in our phonon spectrum analysis by adding an on-site potential quadratic in the displacement. This modifies the phonon spectrum by lifting the low energy modes to finite values. Our analysis clearly indicates that it is primarily the high-energy phonons that are responsible for the superconducting instability. Thus, we do not expect a slight alteration of the low-energy phonon-modes to significantly impact our results. Since the introduction of a substrate may break the $z \rightarrow -z$ mirror symmetry of the system, the out-of-plane modes could potentially also give some contribution to the effective potential, but we expect this to be a higher order effect in the lattice site deviations. A substrate would also affect the Coulomb interaction screening length, thus altering the relative strength of the interaction parameters $\lambda_\nu$. We would expect this to reduce the effect of the Coulomb interaction.

Finally, we note that superconductivity in doped graphene in the presence of Coulomb interaction also has been studied in Refs. 52 and 53 using strong coupling Eliashberg theory with somewhat different approaches for the Coulomb interaction and electron-phonon coupling. These works obtain similar results.

VII. BORON NITRIDE

So far, we have only considered graphene, but our methodology can easily be carried over to other graphene-like materials. In particular, we consider hexagonal boron nitride (h-BN), which is a two-dimensional material very similar to graphene, but where
FIG. 9. (a) Electron spectrum for the $\pi$-band of hexagonal boron nitride (h-BN) in a tight binding hopping model. Contrary to graphene, the band structure is gapped due to sublattice asymmetry. (b) Phonon spectrum for free-standing h-BN in force constant model. In-plane modes are shown in blue, with out-of-plane modes in green.

FIG. 10. Electron-phonon coupling strength $\lambda$ for boron nitride averaged over the Fermi surface at chemical potential $\mu$. The contributions to the total electron-phonon coupling (black) from the various phonon modes is shown in colors. The density of states is shown in magenta. A given energy doping $\mu$ corresponds to a charge doping $n$ per site, and the inset shows the electron-phonon coupling as function of this charge doping for graphene and boron nitride.

In light of these results, we would expect the difficulty of realizing intrinsic phonon-mediated superconductivity in boron nitride to be similar to graphene. Furthermore, the importance of the electron-phonon coupling matrix element illustrates why it is important to treat the electron-phonon coupling in a detailed manner.

VIII. SUMMARY

In summary, we have studied electron-phonon coupling in graphene and hexagonal boron nitride based on an electron tight-binding and a phonon force constant model giving realistic electron and phonon spectra. The ability to tune the relevant system parameters in this detailed model provides a platform for investigating the superconducting properties of graphene and graphene-like systems.

In graphene, we have identified the phonon modes which couple most strongly to $\pi$-band electrons, which are the electronic states of most relevance for realistic doping levels in graphene. These modes are the high-energy in-plane phonon modes. Solving the gap equation assuming singlet pairing, we find the critical temperature and the superconducting gap structure in the Brillouin zone. Our results show that the gap is close to uniform along the Fermi surface in the absence of a Coulomb interaction. Introducing the Coulomb interaction, however, introduces a slight Fermi surface non-uniformity. Furthermore, we find that the Coulomb interaction gives a very dramatic suppression in the critical temperature, in contrast with the moderate reduction in most normal superconductors. We understand this in terms of the Anderson-Morel model, where the calculated electron-phonon coupling strength and estimates for the renormalization are of the same order. Even if one succeeded in doping graphene so much that the electron-phonon coupling could give rise to superconductivity at experimentally observable temperatures, we therefore expect the Coulomb interaction to prevent the occurrence of the superconducting instability. Enhancing the electron-phonon coupling strength remains important to realize phonon-mediated superconductivity in monolayer graphene, but one cannot make predictions without also discussing the effect of Coulomb interaction.

Motivated by the direct onset of a large density of states in the gapped hexagonal boron nitride, we also calculate the dimensionless electron-phonon coupling there within the same framework. In spite of the large density...
of states, however, the charge doping required to obtain a sizeable electron-phonon coupling is similar to the doping required in graphene since the the electron-phonon coupling matrix element is suppressed due to the small Fermi surface at small charge doping.

IX. ACKNOWLEDGEMENTS

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Appendix A: Electron band structure

To calculate the graphene electron band structure, we use the nearest neighbour tight binding Hamiltonian [4],

\[ H_{el} = -t_1 \sum_{\langle ij \rangle} \left( c_i^\dagger c_j + \text{h.c.} \right), \tag{A1} \]

as our starting point. By introducing the Fourier transformed operators, this model becomes

\[ H_{el} = \sum_k \left( c_k^\dagger \epsilon_k c_k \right) M_k \left( c_k A \right), \tag{A2} \]

where the matrix \( M_k \) is given by

\[ M_k = \begin{pmatrix} 0 & -t_1 \sum_\delta \epsilon_{\delta} e^{-ik\delta} \\ -t_1 \sum_\delta \epsilon_{\delta} e^{ik\delta} & 0 \end{pmatrix}, \tag{A3} \]

and \( \delta \) are the nearest neighbour vectors from sublattice \( A \) to sublattice \( B \). Diagonalizing this matrix, we get eigenvectors \( F_\eta(k) \) for the two eigenvalues \( \epsilon_\eta \) corresponding to the two \( \pi \)-bands, where \( \eta \) is the band index. Thus, the \( D \)-sublattice Fourier mode is given by

\[ \alpha_{k\eta} = \sum_k F_{D\eta}(k) \epsilon_k \eta, \tag{A4} \]

where \( \eta \) is the band and an eigenvector of the matrix \( M_k \). This equation provides the definition of the factors \( F_{D\eta}(k) \) appearing in the main text.

Appendix B: Phonon model diagonalization

The phonon dispersion relation calculation in this paper follows Refs. [61] and [62] where the phonon excitation spectrum is calculated for graphene. We take the same approach, and use a force constant model with with up to third nearest neighbour interactions to calculate the dispersion relations for graphene and boron nitride. Since boron nitride has a broken sublattice symmetry, we have to account for the different sublattice masses, and the intersublattice force constants become sublattice dependent. In this Appendix, we discuss how the force constant model can be diagonalized, leaving the discussion of the force constants and their symmetry relations to Appendix C.

We write the phonon Hamiltonian on the form

\[ H_{ph} = \sum_j \left( \frac{P_j^2}{2M_j} + \frac{1}{2} \sum_{i,j} \Phi_{\mu\nu}^{\kappa'\kappa} \left( \delta_{ij} \right) u_{i\mu}^{\kappa'} u_{j\nu}^{\kappa} \right), \tag{B1} \]

where \( i, j \) are lattice site indices on the honeycomb lattice, \( \kappa, \kappa' \) are the corresponding sublattices, \( \mu, \nu \) are Cartesian indices, and \( u_{i\mu}^{\kappa} \) is the deviation of site \( i \) on the sublattice \( \kappa \) (uniquely determined by \( i \)) in direction \( \mu \). The deviation coupling constants are \( \Phi_{\mu\nu}^{\kappa'\kappa} \left( \delta_{ij} \right) \). In the kinetic term, \( P_j \) is the momentum of the particle at site \( j \), and \( M_j \) is the mass.

We next express the phonon Hamiltonian in terms of uncoupled harmonic oscillators. To do this, we first symmetrize the sublattice sectors of the kinetic term. Introducing effective mass \( M = \sqrt{M_A M_B} \) and relative masses \( \mu_D \) given by \( M_D = \mu_D M \), we introduce rescaled deviations and momenta

\[ \tilde{P}_D = P_D / \sqrt{\mu_D} \quad \tilde{u}^D = u^D / \sqrt{\mu_D}, \tag{B2} \]

where the rescaling of the deviations is chosen to retain the canonical commutation relations \( [u_{i\mu}^{\kappa}, P_{j\nu}^{\kappa'}] = i\hbar \delta_{ij} \delta_{\mu\nu} \). Note that this rescaling is trivial in the graphene case since then, \( \mu_A = \mu_B = 1 \). To proceed, we rewrite the Hamiltonian in Fourier space, obtaining

\[ H_{ph} = \frac{1}{2M} \sum_{\kappa, \eta} \tilde{P}_{\kappa} \tilde{P}_{\eta} + \frac{1}{2} \sum_{\kappa, \eta} \sum_{\mu, \nu} D_{\mu\nu}^{\kappa\kappa'}(\eta) \tilde{u}_{\kappa, \mu}^{\kappa'} \tilde{u}_{\eta, \nu}^{\kappa}, \tag{B3} \]

where \( \kappa, \kappa' \) are sublattice indices and the matrix elements \( D_{\mu\nu}^{\kappa\kappa'}(\eta) \) are given by

\[ D_{\mu\nu}^{\kappa\kappa'}(\eta) = \frac{1}{\sqrt{M_A M_B}} \sum_{\delta} \Phi_{\mu\nu}^{\kappa'\kappa} \left( \delta_{ij} \right) e^{i\eta \delta_{ij}}, \tag{B4} \]

where \( \delta_{ij}^D \) is the vector from a lattice site on \( D \)-sublattice to lattice site \( j \) on sublattice \( \kappa' \).

Using the symmetries of the system, as discussed further in Appendix C, the number of independent real
space coupling constants can be reduced drastically. Here, we only point out the effect of the mirror symmetry under \(z \to -z\). Considering the lattice deviation coupling term in the phonon Hamiltonian, this symmetry implies that there cannot be any coupling between the in-plane and the out-of-plane modes, and hence that the phonon eigenmodes are either purely in-plane or out-of-plane. The potential energy term can thus be written on the form \(V_{\text{ph}} = V_{\text{ph}}^x + V_{\text{ph}}^z\), where

\[
V_{\text{ph}}^x = \frac{1}{2} \sum_q \left( \mathbf{u}_{qz}^T \right) \mathbf{M}_q^x \mathbf{u}_{qz}^z = \frac{1}{2} \sum_q \left( \mathbf{u}_{qx}^T \right) \mathbf{M}_q^x \mathbf{u}_{qx}^x
\]

\[
V_{\text{ph}}^z = \frac{1}{2} \sum_q \left( \mathbf{u}_{qz}^x \right) \mathbf{M}_q^z \mathbf{u}_{qz}^x
\]

and the deviations \(\mathbf{u}_q\) are given by

\[
\mathbf{u}_q^z = \left( \mathbf{v}_q^A \mathbf{B}_q \right)^T
\]

\[
\mathbf{u}_q^x = \left( \mathbf{v}_q^A \mathbf{B}_q \right)^T
\]

The matrices \(\mathbf{M}_q^x\) and \(\mathbf{M}_q^z\) are \(2 \times 2\) and \(4 \times 4\) matrices, and the matrix elements for graphene are given in Ref. [61].

For the boron nitride case, similar expressions are derived by inserting values for the coupling constants using the symmetry relations and force constants in Appendix C.

To obtain a system of uncoupled harmonic oscillators, we introduce a new basis \(\mathbf{v}_q^\mu\) given by

\[
\mathbf{v}_q^\mu = \sum_\nu [\mathbf{e}_\nu^D(q)]_{\nu\mu} \mathbf{v}_q^\nu
\]

in which the phonon potential energy is diagonal. Here, \([\mathbf{e}_\nu(q)]_{\mu}\) is given by the eigenvectors of \(\mathbf{M}_k\), \(\nu\) is an eigenvector label, \(\mathbf{e}_\nu^D(q)\) is the phonon polarization vector on sublattice \(D\) at quasimomentum \(\mathbf{q}\), and the index \(\mu\) picks out a Cartesian component. This relation provides a definition for the phonon polarization vectors occurring in the electron-phonon coupling in the main text.

Since the kinetic term remains diagonal in the new basis, the system is reduced to a system of uncoupled harmonic oscillators, from which we obtain the excitation spectrum [72].

In our paper, the phonon spectrum and associated polarization vectors \(\mathbf{e}_\nu^D(q)\) are determined using numerical diagonalization. At the high symmetry point \(K\), one may derive reasonably simple expressions for the eigenfrequencies.

### Appendix C: Boron nitride force constants and symmetry relations

The discussion in this Appendix is a generalization of the graphene force constant model in Refs. [61] and [62] to the case of honeycomb lattices without sublattice symmetry. We provide an overview of how the symmetries of the system impose relations between the force constants in the model, and determine the force constants by fitting the force constant dispersion relation to density functional theory results in Ref. [58].

1. Chiral basis and double counting

Before discussing the symmetries, we make a few remarks about the Hamiltonian on the form

\[
H_{\text{ph}} = \sum_j \frac{\mathbf{P}_j^2}{2M_j} + \frac{1}{2} \sum_{i,j} \sum_{\mu\nu} \Phi_{\mu\nu}^{\kappa\kappa_1}(\delta_{ij}) \mathbf{u}_{\mu_i}^{\kappa_1} \mathbf{u}_{\nu_j}^{\kappa_1}.
\]

Here, \(\sum_i\) denotes the sum over all lattice sites \(i\) on the honeycomb lattice. Hence, all bonds \((i,j)\) are being double counted in the above expression, and we get two contributions for each bond. To symmetrize these contributions, we may therefore impose

\[
\Phi_{\mu\nu}^{\kappa\kappa_1}(\delta_{ij}) = \Phi_{\nu\mu}^{\kappa\kappa_1}(\delta_{ij})
\]

Initially, we consider the indices \(\mu,\nu\) to be Cartesian indices. The Hamiltonian may however also be expressed in terms of a chiral basis

\[
\xi = x + iy \quad \eta = x - iy,
\]

so that \(\mu, \nu \in \{\xi, \eta, z\}\). The advantage of this basis is that under a rotation with angle \(\phi\) around the \(z\)-axis, the new coordinates do not mix, and transform according to

\[
\xi \to \xi e^{i\phi} \quad \eta \to \eta e^{-i\phi}.
\]

This comes in handy when utilizing \(C_3\) rotation symmetry to relate bond coefficients.

In terms of the old coupling coefficients, the coefficients for the deviations in the new basis are given by

\[
\Phi_{\xi\xi} = \left( \Phi_{xx} - \Phi_{yy} - i \Phi_{xy} - i \Phi_{yx} \right) / 4
\]

\[
\Phi_{\eta\eta} = \left( \Phi_{xx} - \Phi_{yy} + i \Phi_{xy} + i \Phi_{yx} \right) / 4
\]

\[
\Phi_{\xi\eta} = \left( \Phi_{xx} + \Phi_{yy} + i \Phi_{xy} - i \Phi_{yx} \right) / 4
\]

(\(C4\))

Now, both the deviations and coupling constant are complex. The potential energy itself must however still be real, and this imposes another condition on the coupling constants, in addition to the symmetries mentioned previously.

2. Force constant symmetry relations

The hexagonal boron nitride system has infinitesimal translation symmetry, Bravais lattice translation symmetry, infinitesimal rotation symmetry, lattice \(C_3\) rotation
symmetry, $\sigma_z$ mirror symmetry, and, with our choice of lattice orientation, $\sigma_x$ mirror symmetry. We use these symmetries to reduce the number of independent coupling coefficients.

a. Translation symmetries

From translation symmetry with a Bravais lattice vector $a$, it follows trivially, as already indicated by the force constant notation, that

$$\Phi_{\mu\nu}^{c_i c_j}(\delta_{ij}) = \Phi_{\mu\nu}^{c_i c_j}(\delta_{i+\alpha_j+a}).$$  \hspace{1cm} (C5)

Due to the infinitesimal translation translation symmetry of a single graphene sheet under $u_{i\mu}^{c_i} \rightarrow u_{i\mu}^{c_i} + a_{\mu}$, it furthermore follows that

$$\sum_j \Phi_{\mu\nu}^{c_i c_j}(\delta_{ij}) = 0.$$  \hspace{1cm} (C6)

Following Refs. 61 and 62, we call this the stability condition, and use it to determine the local force constants with $\delta_{ij} = 0$.

Although infinitesimal lattice translation symmetry holds for a freestanding graphene sheet, it breaks down if the monolayer sheet is placed on a substrate. This would give rise to additional free parameters through the force constants $\Phi_{\mu\nu}^{D_D}(0)$.

b. Rotation symmetries

Application of the $C_3$-symmetry under 3-fold rotations $R_3$ gives force constant relations

$$\Phi_{\mu\nu}^{c_i c_j}(R_3\delta_{ij}) = \Phi_{\mu\nu}^{c_i c_j}(\delta_{ij}) \exp(i2\pi/3),$$  \hspace{1cm} (C7)

whereas $\Phi_{\mu\nu}^{c_i c_j}(R_3\delta_{ij}) = \Phi_{\mu\nu}^{c_i c_j}(\delta_{ij}) \exp(-i2\pi/3)$, and this can be combined with the above mirror symmetry $\sigma_z$ to obtain

$$\Phi_{\mu\nu}^{c_i c_j}(\delta_{ij}) = \Phi_{\mu\nu}^{c_i c_j}(\sigma_z \delta_{ij}).$$  \hspace{1cm} (C9)

As already discussed in Appendix B, this is an important symmetry because it completely decouples the in-plane and the out-of-plane phonon modes, and allows us to think of them completely independently.

Furthermore, with our lattice orientation, we have a $\sigma_x$ mirror symmetry. This symmetry implies

$$\Phi_{\mu\nu}^{c_i c_j}(\delta_{ij}) = \Phi_{\mu\nu}^{c_i c_j}(\delta_{ij})^*.$$  \hspace{1cm} (C10)

Finally, we note that the requirement of a real potential gives the relation

$$\Phi_{\mu\nu}^{c_i c_j}(\delta_{ij}) = \Phi_{\mu\nu}^{c_i c_j}(\sigma_x \delta_{ij}).$$  \hspace{1cm} (C11)

For the case of neighbor vectors parallel to the y-axis, invariance of the neighbour vector under the mirror symmetry $\sigma_x$ implies that the coupling constant has to be real.

3. Boron nitride force constants

Applying the above symmetry relations, the independent force constants in the system are listed in Table I along the bonds illustrated in Fig. 11. The other force constants in the system up to next-to-nearest neighbour can be determined from the force constant symmetry relations listed above. Note that, contrary to what Refs. 31 and 32 claim, the force constants $\gamma_{1D}$ are in general complex, whereas the other independent force constants to third-nearest-neighbour order, including $\delta_{1D}$, are real.
The tabulated values give $\Phi/\hbar$ in spectroscopic units of $10^5$ cm$^{-1}$, related to frequency through a factor $2\pi c$, where $c$ is the speed of light.

| Parameter | Coupling | R/C Graphene | k-BN |
|-----------|----------|--------------|------|
| $\alpha$ | $\Phi_{CB}^B(\alpha_1)$ | R | -4.046 | -3.15 |
| $\beta$ | $\Phi_{CB}^B(\alpha_1)$ | R | 1.107 | 1.69 |
| $\gamma_A$ | $\Phi_{\xi\eta}^A(\beta_1)$ | C | -0.238 | -0.32 + 0.05i |
| $\gamma_B$ | $\Phi_{\xi\eta}^B(\beta_1)$ | C | -0.238 | -0.36 - 0.07i |
| $\delta_A$ | $\Phi_{\xi\eta}^A(\beta_1)$ | R | -1.096 | -0.68 |
| $\delta_B$ | $\Phi_{\xi\eta}^B(\beta_1)$ | R | -1.096 | -0.66 |
| $\alpha'$ | $\Phi_{\xi\eta}^A(\gamma_1)$ | R | - | 0.00 |
| $\beta'$ | $\Phi_{\xi\eta}^B(\gamma_1)$ | R | - | -0.23 |
| $\alpha_z$ | $\Phi_{\xi\eta}^B(\alpha_1)$ | R | -1.176 | -1.06 |
| $\gamma_A'$ | $\Phi_{\xi\eta}^A(\beta_1)$ | R | 0.190 | 0.00 |
| $\gamma_B'$ | $\Phi_{\xi\eta}^B(\beta_1)$ | R | 0.190 | 0.24 |

where $u_n$ is the interaction strength, and $\sigma, \sigma'$ are spin indices. The index $D \in \{A, B\}$ is a sublattice index, whereas $\tilde{D}_n = D$ if the $n$-th nearest neighbour of a given lattice site is on the same sublattice (i.e. intra-sublattice interaction) and $\tilde{D}_n \neq D$ otherwise (inter-sublattice interaction). The set of vectors $\{\delta_D^n\}$ are the $n$-th nearest neighbour vectors from sublattice $D$ to sublattice $\tilde{D}_n$. The Kronecker-delta factor $(1 - \delta_{\sigma\sigma'}\delta_{n,0})$ is introduced to ensure that there is no on-site intra-spin contribution. Expressing the interaction in terms of the band eigenvalues then gives

$$V_{C,n}^D = \frac{u_n}{2N_A} \sum_D \sum_{\sigma\sigma'} \sum_{kkq} (1 - \delta_{\sigma\sigma'}\delta_{n,0}) \left( \sum_{\delta_D^n} \epsilon_q \delta_{\sigma\sigma'}^{\delta_D^n} \right) F_{D\eta_1\eta_2\eta_3}(k + q) F_{D\eta_1\eta_2\eta_3}'(k' - q) F_{D\eta_4}(k') F_{D\eta_4}(k) c_{\eta_1\sigma}(k + q) c_{\eta_2\sigma'}(k' - q) c_{\eta_3\sigma'}(k) c_{\eta_4\sigma}(k),$$

specialization, the potential takes the form

$$V_{C,n}^D = \sum_{kk'} V_{kk'}^{C,n} c_{\eta_1}(k) c_{\eta_1}(k') c_{\eta_1}(k) c_{\eta_1}(k'),$$

and one can read off the BCS singlet pairing effective potential contribution from the $n$-th nearest neighbour interaction from the explicit expression for $V_{kk'}^{C,n}$. The scattering amplitudes $E_{\eta_1\eta_2}(k, k')$ are then given by

In this Appendix, starting from the real space Coulomb interaction expression in Eq. (6), we derive the structure factors of Eq. (9). This is done by first expressing the interaction in terms of Fourier sublattice modes, which are subsequently replaced with the band eigenmodes. The pairing potentials occurring in the BCS gap equation can then be read off by specializing the potential to the quasi-momenta, spins and band indices corresponding to BCS singlet pairing.

In terms of the sublattice Fourier modes, the interaction term corresponding to the $n$-th nearest neighbour is given by

$$V_{C,n}^D = \frac{u_n}{2N_A} \sum_D \sum_{\sigma\sigma'} \sum_{kkq} (1 - \delta_{\sigma\sigma'}\delta_{n,0}) \left( \sum_{\delta_D^n} \epsilon_q \delta_{\sigma\sigma'}^{\delta_D^n} \right) F_{D\eta_1}(k + q) F_{D\eta_2}(k' - q) F_{D\eta_3}(k') F_{D\eta_4}(k) c_{\eta_1\sigma}(k + q) c_{\eta_2\sigma'}(k' - q) c_{\eta_3\sigma'}(k) c_{\eta_4\sigma}(k),$$

where $\eta_i$ are band indices and the coefficients $F_{D\eta_i}$ are discussed in the main text and Appendix A. Finally, we specialize to BCS singlet pairing by letting $k = -k$, considering scattering within a single band $\eta$ and considering spins $\sigma = -\sigma'$. For the case of intra-sublattice interaction, this leads to complete cancellation of the prefactors $F_{D\eta}$ by using $F_{D\eta}(k) F_{D\eta}(-k) = 1/2$, and consequently, the resulting effective interaction depends only on the scattering quasimomentum $q$. For the inter-sublattice interaction, there is no such cancellation, and the effective potential retains a more convoluted form. After this

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where \( \mathbf{q} = \mathbf{k}' - \mathbf{k} \) and one has to choose expression based on whether \( n \) denotes an on-site, inter- or intra-sublattice contribution.

**Appendix E: Numerical details of solving the gap equation**

The gap equation is given by

\[
\Delta_k = -\frac{1}{N_A} \sum_{k'} \tilde{\gamma}_{kk'}^{\text{symm}} \chi_{k'} \Delta_{k'}
\]  

where \( N_A \) is the Brillouin zone area and we let \( \tilde{\gamma}_{kk'}^{\text{symm}} = N_A V_{kk'}^{\text{symm}} \).

To find a proper solution to the gap equation, it is important to have sufficiently good resolution in the important regions of the Brillouin zone. The factor \( \chi_{k} \) is peaked around the Fermi surface with a peak width \( \propto T \) and necessitates a good resolution there. Furthermore, good resolution is also required in the regions around the corners of the triangle-like Fermi surface at significant doping. To make sure of this, we select points on a uniform grid in the Brillouin zone, add additional points close to the Fermi surface, and further additional points close to the Fermi surface corners.

To solve the gap equation, we rewrite the gap equation on the integral form (E2) in terms of a weighted sum over the points described in the previous paragraph. To find the appropriate weights \( \omega_{k} \), we split the Brillouin zone into triangles \( \{ t \} \) with the points \( \{ \mathbf{k} \} \) as vertices using Delaunay triangulation. Denote the area of a triangle \( t \) by \( A_t \). The weight of a single point then becomes one third of the sum of the areas of all the triangles that has the point as a vertex, i.e.

\[
\omega_{k} = \sum_{t} A_t \delta_{k t}/3,
\]  

where \( \delta_{k t} \) is 1 if \( \mathbf{k} \) is a vertex in the triangle \( t \) and 0 otherwise.

The gap equation then becomes

\[
\Delta_k = -\frac{1}{A_{BZ}} \sum_{k'} \tilde{\gamma}_{kk'}^{\text{symm}} \omega_{k} \chi_{k} \Delta_{k'}
\]  

where we introduced the weighted gap \( \hat{\Delta}_k = \sqrt{\omega_k \chi_k} \Delta_k \), and the matrix

\[
M_{kk'} = -\frac{1}{A_{BZ}} \left( \sqrt{\omega_k \chi_k} \tilde{\gamma}_{kk'}^{\text{symm}} \sqrt{\omega_{k'} \chi_{k'}} \right)
\]  

is symmetric in the interchange of \( \mathbf{k} \) and \( \mathbf{k}' \). This symmetrization allows faster computation of the eigenvalues and eigenvectors.

We now have a matrix eigenvalue problem linear in the eigenvectors and non-linear in the eigenvalue. To find the gap structure at the superconducting instability by determining the smallest \( \beta \), i.e. the largest temperature, for which the largest eigenvalue of \( M_{kk'} \) becomes 1. The corresponding eigenvector must be a solution of our eigenvalue problem. Location of the critical temperature \( T_c = 1/\beta_c \) is done using the bisection method.

**Appendix F: Parameter values**

The parameter values used in the electron tight binding model and the electron-phonon coupling for graphene and boron nitride are listed in Table III. The electron-phonon coupling scale \( g_0 \) can be written as

\[
g_0 = \gamma t_1 \sqrt{\frac{\hbar^2}{2m_e a_0^2}} \frac{1}{\hbar \omega_T} \left( \frac{m_e}{M} \right) \left( \frac{a_0}{d} \right)^2,
\]  

where \( m_e \) is the electron mass, and \( a_0 \) the Bohr radius. This quantity is calculated based on the listed parameter values, and also given in the table.
TABLE II. Values for the quantities involved in the calculation of the electron-phonon coupling amplitude strength $g_0$, where the A-sublattice of boron nitride is assumed to host boron and the B-sublattice nitrogen.

| Quantity | Graphene | h-BN | Description |
|----------|----------|------|-------------|
| $d$      | 1.42 Å   | 1.45 Å | NN-distance |
| $t_1$    | 2.8 eV | 2.92 eV | Hopping amplitude |
| $\Delta$ | 0      | 4.30 eV | Band gap |
| $\hbar \omega_c$ | 0.20 eV | 0.17 eV | Phonon energy scale |
| $M$      | 12.0 u  | 12.3 u | Effective mass |
| $\mu_A$  | 1       | 0.88   | Relative mass, A-subl. |
| $\mu_B$  | 1       | 1.14   | Relative mass, B-subl. |
| $\gamma$ | 5       | 5      | $-d \log t_1/d \log d$ |
| $m_e$    | $5.49 \cdot 10^{-4}$ u | Electron mass |
| $\xi$    | 13.6 eV | Rydberg energy |
| $a_0$    | 0.53 Å  | Bohr radius |
| $g_0$    | 0.29 eV | 0.31 eV | El-ph coupling scale |

### Appendix G: Anderson-Morel model

The Anderson-Morel model is a simple model describing the effect of a repulsive potential in the entire Brillouin zone on top of an attractive potential in a small region around the Fermi surface giving rise to superconductive pairing [29]. This model illustrates why there can be a superconducting instability even though the interaction potential strengths for our Coulomb interaction lattice model, we fit the critical temperature to a function on the form

$$k_B T_c = 1.14 \hbar \omega_D \exp \left\{ -\frac{1}{\lambda - \mu^*} \right\},$$

where

$$\mu^* = \frac{\tilde{u}}{1 + \tilde{u} \log(W/\hbar \omega_D)}$$

is the renormalization due to the presence of the repulsive interaction, $\tilde{u} = N_0 u$ is a dimensionless measure of the repulsive interaction, and $\lambda = N_0 v$ is the potential strength of the attractive potential. The effect of the repulsive Coulomb potential is therefore to renormalize the strength $\lambda$ of the attractive potential in the critical temperature formula. At sufficiently large renormalization $(\mu^* \geq \lambda)$, the analysis breaks down, and there is no superconducting instability.

After solving the gap equation with different overall potential strengths for our Coulomb interaction lattice model, we fit the critical temperature to a function on the form

$$k_B T_c = 1.14 \hbar \omega_D \exp \left\{ -\frac{1}{\lambda - \frac{a}{1 + abu}} \right\},$$

with two fitting parameters $a$ and $b$ in addition to the electron-phonon coupling strength $\lambda$, which is fixed by the critical temperature at zero repulsive Coulomb interaction.

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