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Pauli limiting and metastability regions of superconducting graphene and intercalated graphite superconductors

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Abstract:
We present a study of metastability regions in the in-plane magnetic field *vs.* temperature phase diagram of graphene and intercalated graphite superconductors. Due to the vanishing density of states, undoped graphene requires a finite BCS interaction V_c to become superconducting (any finite doping drives this critical value to zero). Above V_c , superconducting graphene under in-plane magnetic field displays the conventional low temperature first-order transition (FOT) to the normal phase, but the width of the associated metastability region (normalized to the zero temperature critical field) vanishes when doping goes to zero and the interaction approaches V_c . In the case of intercalated graphite superconductors, modeled as two-dimensional two-band superconductors (a graphene-like band and a metallic interlayer band), a critical graphene intraband interaction is required in order for the appearance of a second metastability region in the superconducting region of the phase diagram. The width of this metastability region also goes to zero as the graphene intraband interaction approaches, from above, its critical value and the metastability region vanishes at the zero temperature supercooling field associated to the metallic interlayer band. Slightly above this critical value, the low-temperature FOT line bifurcates at an intermediate temperature into a FOT line and a second-order transition line.

Graphene lattice and density of states (DOS)

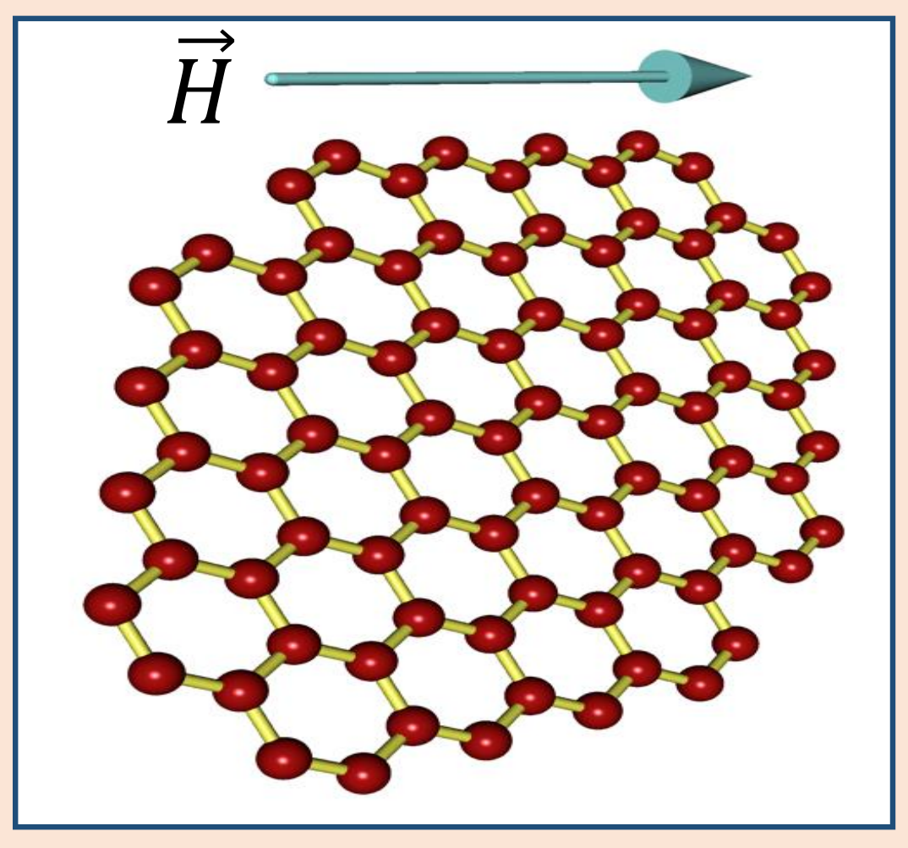

Fig. 1: Illustration of a graphene sheet with a periodic honeycomb lattice of carbon atoms (red spheres), under an in-plane magnetic field (light blue arrow).

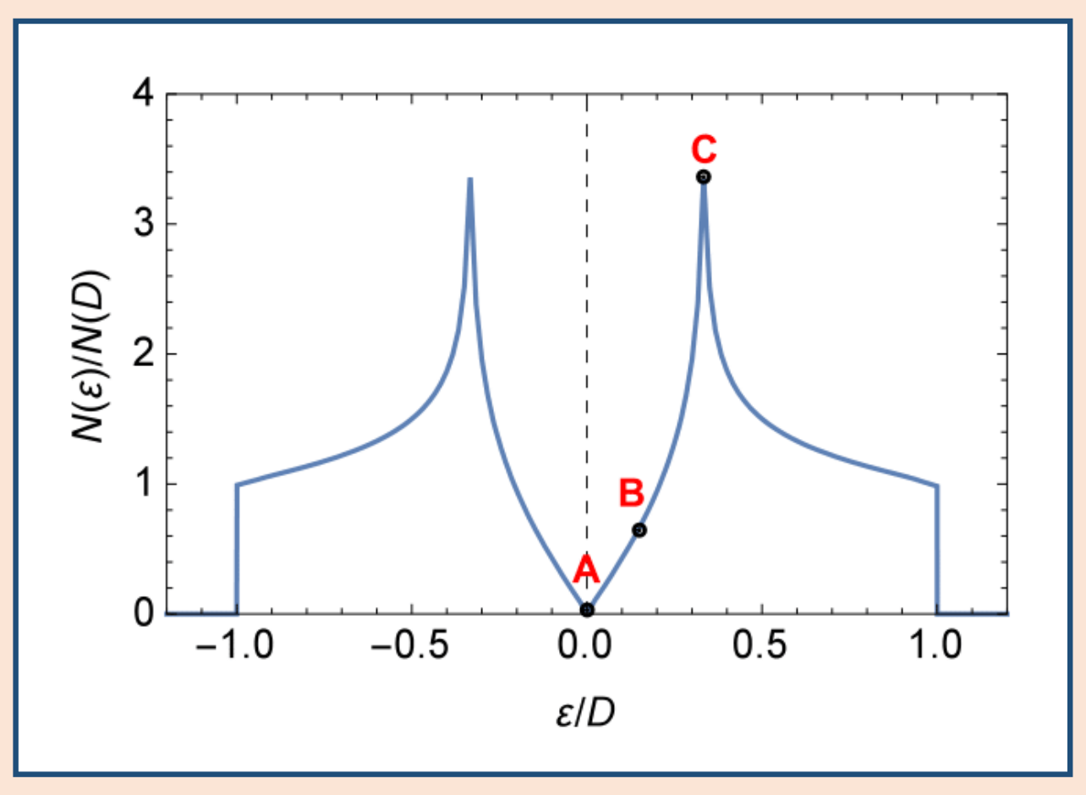

Fig. 2: DOS of graphene (normalized to its value at the half-bandwidth D) as a function of energy (normalized to D).

Hamiltonian and band-gap equations

Hamiltonian of a *n*-band superconductor in the weak-coupling limit (introduced by Sulh, Matthias and Walker), with a Zeeman splitting term:

$$\begin{aligned}\mathcal{H} - \mu\mathcal{N} - \sigma h\mathcal{N} &= \sum_{\mathbf{k}\sigma i} \xi_{\mathbf{k}\sigma i} c^{\dagger}_{\mathbf{k}\sigma i} c_{\mathbf{k}\sigma i} \\ &- \sum_{\mathbf{k}\mathbf{k}' ij} V^{ij}_{\mathbf{k}\mathbf{k}'} c^{\dagger}_{\mathbf{k}\uparrow j} c^{\dagger}_{-\mathbf{k}\downarrow j} c_{\mathbf{k}'\uparrow i} c_{-\mathbf{k}'\downarrow i}\end{aligned}$$

where $\mathrm{i,j} = 1{,}2$ is the band index in the case of a two-band superconductor ($\mathrm{i,j} = 1$ in the case of a one-band superconductor), μ is the chemical potential, $\sigma = \uparrow, \downarrow$ is the spin component along the in-plane magnetic field, $h = \mu_B H$, μ_B and H are the Bohr magneton and the in-plane applied magnetic field, respectively, $\xi_{k\sigma i} = \varepsilon_{ki} - \mu - \sigma h$ is the kinetic energy term measured from μ, and $V^{ij}_{\boldsymbol{kk'}}$ gives the intraband ($i = j$) and interband ($i \neq j$) pairing interactions.

Applying the mean field approach to this Hamiltonian, and minimizing the respective free energy with respect to the superconducting gaps, one obtains an expression for the coupled superconducting gap equations, where *s*-wave symmetry is assumed,

$$\Delta_i = \sum_j V_{ij}\delta_j,$$

with

$$\begin{aligned}\delta_j &= \delta_j(T, h, \Delta_j, N_j(\xi)) \\ &= \int_0^{\omega_D} d\xi \Delta_j \frac{N_j(\xi)}{2E_j}\left(\tanh\frac{E_j + h}{2k_BT} + \tanh\frac{E_j - h}{2k_BT}\right),\end{aligned}$$

and where $E_j = \sqrt{\xi^2 + \Delta_j^2}$ is the quasi-particle excitation energy of the j band, ω_D is the usual frequency cutoff, $N_j(\xi)$ is the DOS of the j band, T is the temperature and k_B is the Boltzmann constant. In the case of a one-band superconductor, one has a single gap equation ($i = 1$ and $j = 1$).

GIC's modeled as two-dimensional two-band superconductors

- Highly anisotropic graphite intercalation compounds (GIC's) modeled as two-dimensional two-band superconductors where one of the bands is treated as a graphene-like band and the other as a generic 2D metallic band:

$$\begin{pmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{pmatrix} N_1(0) \rightarrow \begin{pmatrix} 0.2 & 0.008 \\ 0.008 & V_{22} \end{pmatrix},$$

where V_{11} is the intraband potential of the metallic interlayer band, V_{22} is the intraband potential of the graphene-like band, $V_{12} = V_{21}$ is the interband potential which couples the two bands, and $N_1(0)$ is the density of states of the metallic band at the Fermi energy.

- Josephson tunneling of Cooper pairs from the metallic band ($V_{12} \neq 0$):

Graphene-like band becomes superconducting (finite Δ_2) for any value of V_{22}, even when $\mu = 0$. **Thus, in this case, there is not a critical value of the graphene-like intraband coupling, V_c.**

However, a new critical intraband coupling V_{c2} for the graphene-like band can be defined, associated with the appearance of a second metastability region in the superconducting phase of the in-plane magnetic field *vs*. temperature phase diagram**.** The second metastability region reflects the existence of intrinsic pairing in the graphene-like band and this requires a finite V_{22}.

Superconductivity in graphene

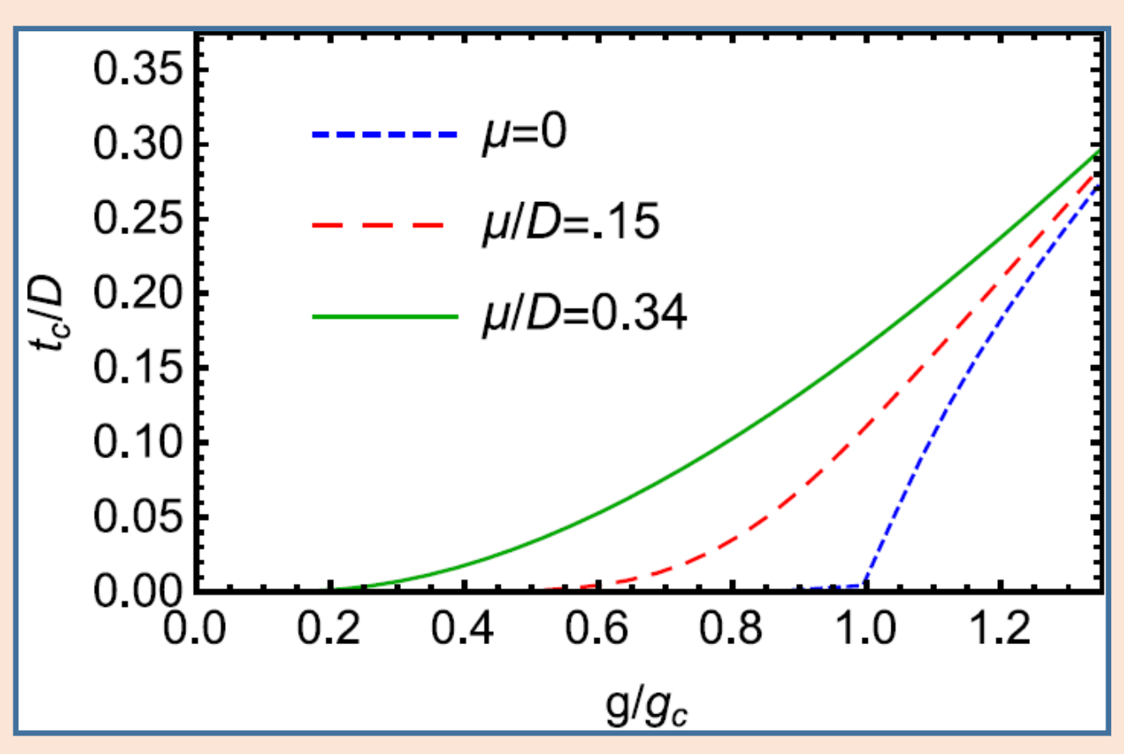

Fig. 3: Critical temperature, t_c, at zero magnetic field as a function of the BCS pairing interaction, V, (normalized to the critical interaction value V_c), for several values of doping, indicated by points A, B, and C in Fig. 2.

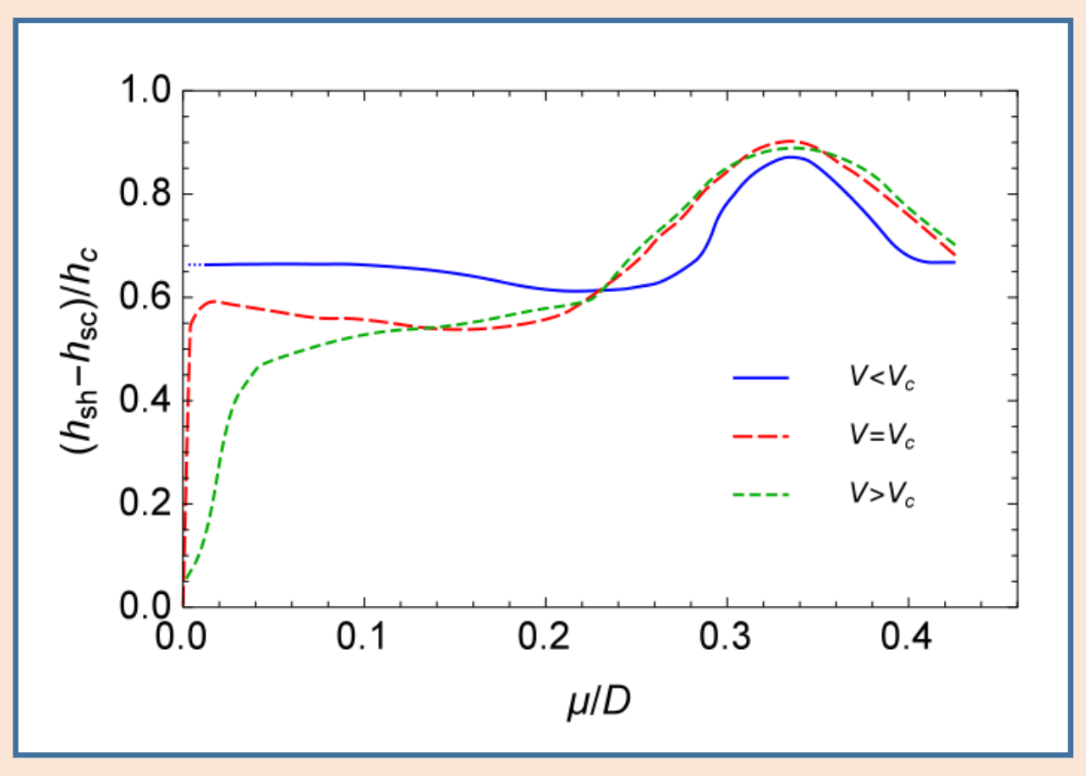

Fig. 4: Zero temperature width (normalized to the zero temperature critical field) behavior of the metastability region with doping, for $V = 0.78V_c$, $V = V_c$, and $V = 1.03V_c$.

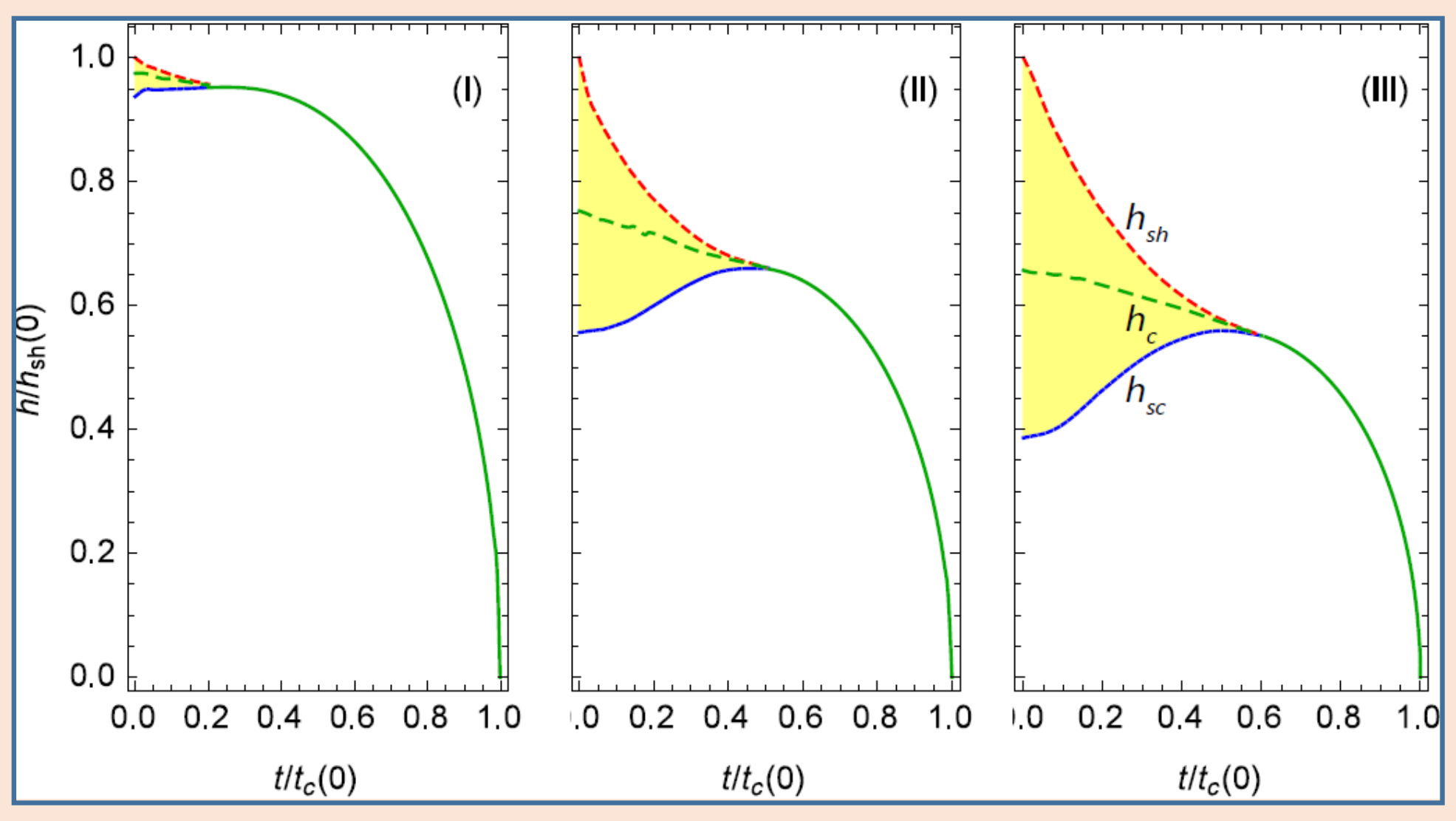

Fig. 5: In-plane magnetic field vs. temperature phase diagram of graphene, for (I) $\mu /D = 0$, (II) $\mu /D = 0.15$, and (III) $\mu /D = 0.34$, for $V = 1.03\,V_c$. For $\mu /D = 0$, the metastability region (yellow shaded area) is very narrow and with doping, from (I) to (III), its normalized width increases as the Fermi energy is shifted away from the Dirac point. Furthermore there is not a universal value for the tricritical temperature, which can take values $T < 0.56T_c(0)$, becoming smaller as $\mu \rightarrow 0$.

Intercalated graphite under in-plane magnetic fields

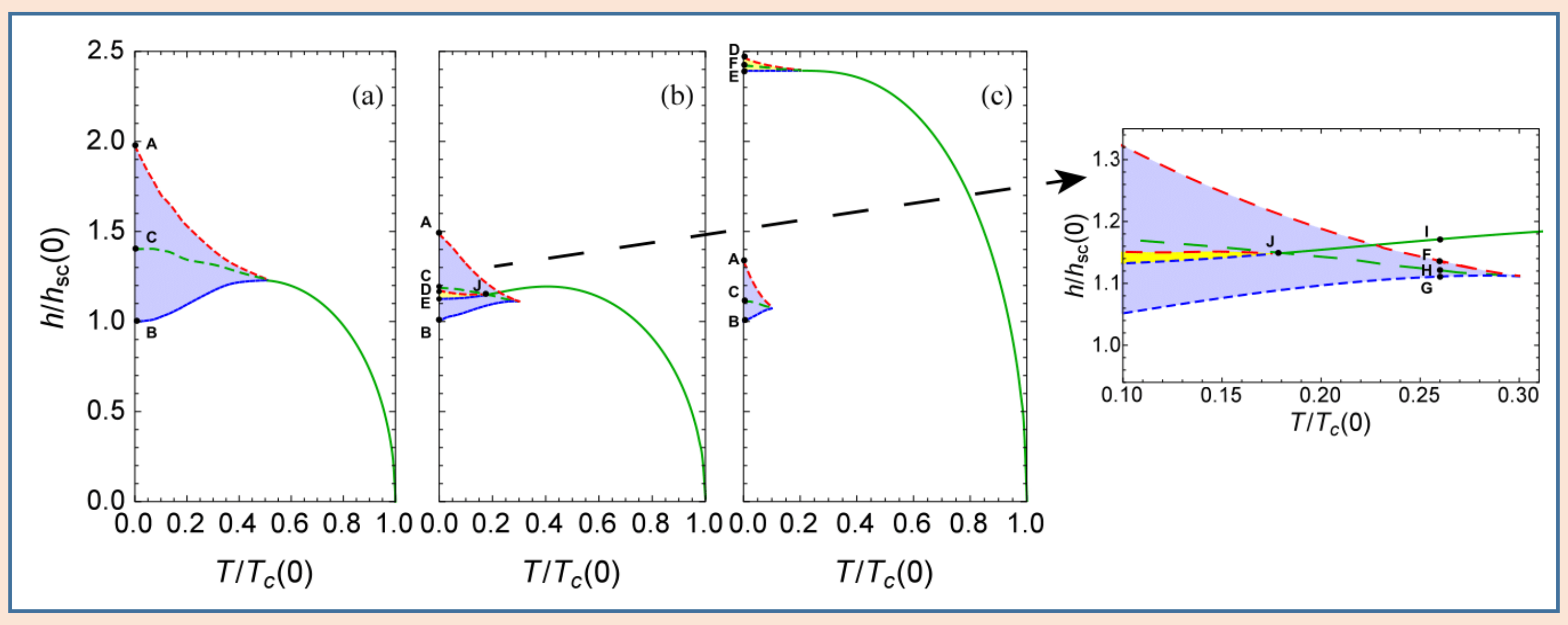

Fig. 6: In-plane magnetic field *vs*. temperature phase diagram of intercalated graphite (using a two-band BCS description) for (a) $V_{22} = 0.18$ ($V_{22} < V_{c2}$), (b) $V_{22} = 0.24$ ($V_{22} \gtrsim V_{c2}$) and (c) $V_{22} = 0.26$ ($V_{22} > V_{c2}$). The metastability region associated primarily with intraband pairing in the metallic (graphene) band is shown in the blue (yellow) shaded area. From (a) to (c) the phase diagram changes from one of a typical one-band to one of a typical two-band superconductor phase diagram. In the intermediate case, (b), unusual behavior occurs: at the zoomed plot of (b) one sees, at a temperature $T \approx 0.175T_c$, that the FOT (dashed green curve C-J) splits into a upper SOT (solid green curve J-I) and an additional lower FOT (dashed green curve J-H).

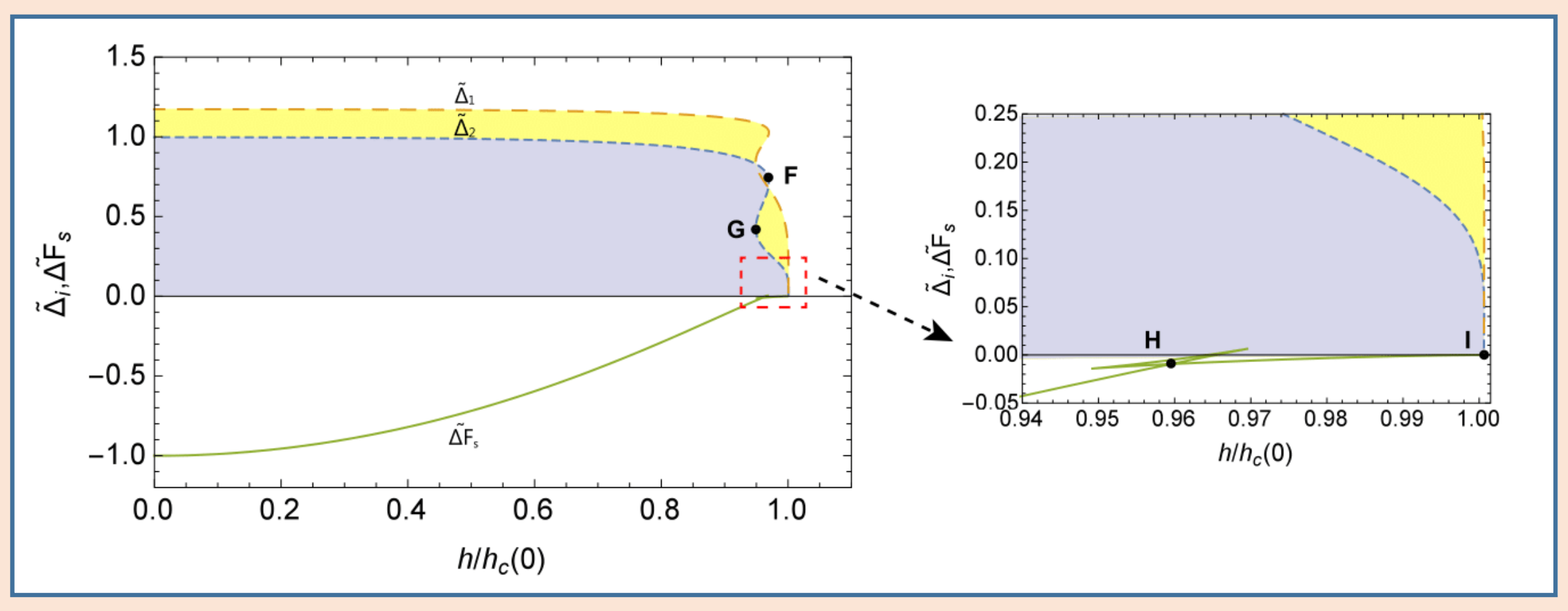

Fig. 7: Solutions of the coupled gap equations and the total free energy difference between the superconducting and the normal phases of a two-band intercalated graphite superconductor at $T = 0.26T_c$ for $V_{22} \gtrsim V_{c2}$ and a zoomed region showing a crossing in the free energy before the SOT to the normal phase. The labeled points correspond to those in Fig. 6.

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