Coupled First-Order Transitions In A Fermi-Bose Mixture

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(Dated: December 3, 2019)

A model of a mixture of spin-zero hardcore bosons and spinless fermions, with filling fractions \(\rho_B\) and \(\rho_F\), respectively, on a two-dimensional square lattice with composite hopping \(t\) is presented. In this model, hopping swaps the locations of a fermion and a boson at nearest-neighbor sites. When \(\rho_B + \rho_F = 1\), the fermion hopping amplitude \(\phi\) and boson superfluid amplitude \(\psi\) are calculated in the ground state within a mean-field approximation. The Fermi sector is insulating \((\phi = 0)\) and the Bose sector is normal \((\psi = 0)\) for \(0 \leq \rho_F < \rho_c\). The model has coupled first-order transitions at \(\rho_F = \rho_c \simeq 0.3\) where both \(\phi\) and \(\psi\) are discontinuous. The Fermi sector is metallic \((\phi > 0)\) and the Bose sector is superfluid \((\psi > 0)\) for \(\rho_c < \rho_F < 1\). At \(\rho_F = 1/2\), fermion density of states \(\rho\) and bulk modulus \(\kappa\) display cusp-like singularities, and \(\phi\) and \(\psi\) are maximum. At \(\rho_F = \rho_c \simeq 0.81\), \(\kappa\) vanishes, becoming negative for \(\rho_c < \rho_F < 1\). The role of composite hopping in the evolution of Fermi band dispersions and Fermi surfaces as a function of \(\rho_F\) is highlighted.

Fermi-Bose mixtures (FBMs) constitute an unusual phase of matter, the earliest examples of which are the mixed phase of type-II superconductors and He\textsuperscript{3}-He\textsuperscript{4} mixtures \cite{1}. In the past two decades, fascinating experiments on FBMs of ultracold atoms have revealed unique properties and given a major thrust to their study \cite{2,3,4}. While superfluidity was observed very early in either the Fermi or Bose sector of an FBM, the coexistence of superfluidity in both sectors was reported very recently \cite{5}.

Theoretical and experimental studies of FBMs have developed significantly over the years, particularly in terms of a crossover between the limiting cases of the BCS picture of superconductivity and the BEC picture of superfluidity \cite{6,7}. The BCS-BEC crossover was predicted to occur for excitons in semiconductors \cite{8}, quarks \cite{9}, and interestingly, it was first realized in ultracold fermionic atoms with s-wave interactions \cite{10}. The growing number of experimental results includes the Feshbach resonance across the BCS-BEC crossover \cite{11}, formation of a Feshbach molecule in an FBM \cite{12}, and the role of three body physics in describing an FBM \cite{13} to name a few. More recently, experimental results of some iron-based superconductors and the relevance of their electronic structure and properties \cite{14,15,16,17} have also been discussed in relation to theoretical results of the BCS-BEC crossover \cite{6,18,19}. While it is well-known that interactions between fermions mediated by phonons are at the root of the BCS theory of superconductivity, several studies have also considered their importance in FBMs of ultracold atoms \cite{20,21,22,23}. The BCS theory was preceded by the so-called Boson-Fermion (BF) model \cite{24}, which discusses itinerant fermions hybridizing with bosons composed of bound pairs of fermions of opposite spins. The BF model was later applied to study electrons interacting with local lattice deformations \cite{25} and high temperature superconductivity \cite{26,27,28,29}. More recently, it was also used for describing resonance superfluids in the BCS-BEC crossover regime \cite{30} as well as a temperature driven BCS-BEC crossover in an FBM \cite{31}. The interplay of bosonic and fermionic degrees of freedom is therefore of great importance in several physical systems.

In this work, we address the coupling of bosonic and fermionic degrees of freedom in a zero-temperature mean-field study of an FBM on a two-dimensional square lattice via composite hopping, with a filling constraint of one particle per site. The model displays two distinct phases separated by coupled first-order transitions at Fermi filling fraction \(\rho_F = \rho_c \simeq 0.3\); for \(\rho_F < \rho_c\), the Fermi sector is insulating and the Bose sector is a normal gas, while for \(\rho_F > \rho_c\), the Fermi sector is metallic and the Bose sector is a superfluid. The fermion band width varies with the Fermi energy. The fermion density of states and bulk modulus exhibit cusp-like singularities at \(\rho_F = 1/2\), and the bulk modulus becomes negative for \(\rho_F > \rho_c \simeq 0.81\). Our estimate of BEC transition temperature in this model is several hundred kelvins.

The Hamiltonian we study is

\[
H = -\alpha \sum_i \left[ b_i^\dagger b_i + f_i^\dagger f_i - 1 \right] - \mu \sum_i f_i^\dagger f_i + \frac{U}{2} \sum_i b_i^\dagger b_i (b_i^\dagger b_i - 1) - t \sum_{\langle ij \rangle} f_i^\dagger f_j b_j^\dagger b_i \tag{1}
\]

where \(b_i^\dagger\) creates a spin-zero boson and \(f_i^\dagger\) creates a spinless fermion at site \(i\) of a two-dimensional square lattice. The parameter \(\alpha\) is a Lagrange multiplier: it is used for imposing the condition that the total number of fermions and bosons be a certain given number (taken to be equal to the number of lattice sites in this work); \(\mu\) is the chemical potential used to determine \(\rho_F\); \(U\) is the repulsive energy between two bosons at the same site; finally, \(t\) is the strenght of the composite hopping: in this process a fermion hops from a site \(j\) to a neighboring site \(i\) when a boson located there simultaneously hops to site \(j\). The boson operators satisfy \([b_i, b_j] = 0 = \ldots\)
$[b_i^\dagger, b_j^\dagger] = \delta_{ij}$, while the spinless-fermion operators satisfy $\{f_i, f_j\} = 0$, $\{f_i^\dagger, f_j^\dagger\} = 0$, $\{f_i, f_j^\dagger\} = \delta_{ij}$, where $[a, b] = ab - ba$ and $[a, b] = ab + ba$. In this paper, we restrict ourselves to hardcore bosons, i.e. the limit $U \to \infty$, and impose the constraint

$$\rho_F + \rho_B = 1, \quad (2)$$

($\rho_B$ is the boson filling fraction) by requiring $\partial F/\partial \alpha = 0$, $F$ being the free energy.

To calculate the properties of the hamiltonian $\hat{H}$, we use the following approximation:

1. If $\hat{F}$ is a fermion operator and $\hat{B}$ is a boson operator, then $\hat{F}\hat{B} \simeq \langle \hat{F}\rangle\hat{B} + \langle \hat{B}\rangle \hat{F} - \langle \hat{F}\rangle\langle \hat{B}\rangle$. 
2. If $\hat{B}_i, \hat{B}_j$ are boson operators at sites $i \neq j$, then $\hat{B}_i\hat{B}_j \simeq \langle \hat{B}_i\rangle\hat{B}_j + \langle \hat{B}_j\rangle\hat{B}_i - \langle \hat{B}_i\rangle\langle \hat{B}_j\rangle$. 

The first step implies $\langle \hat{F}\hat{B}\rangle \simeq \langle \hat{F}\rangle\langle \hat{B}\rangle$, so this is equivalent to factorizing the state space into a product of fermion and boson subspaces. The second step implies $\langle \hat{B}_i\hat{B}_j\rangle \simeq \langle \hat{B}_i\rangle\langle \hat{B}_j\rangle$, which is equivalent to further factorizing the boson subspace into a product of single-site subspaces: this is the standard mean-field decoupling used in the bosonic Hubbard model [32–38]. When we follow these steps, the composite hopping term is transformed according to

$$f_i^\dagger f_j b_j^\dagger b_i \simeq \langle f_i^\dagger f_j\rangle (\langle b_j^\dagger b_i\rangle + \langle b_j\rangle \langle b_i\rangle) + (\langle b_j^\dagger\rangle \langle b_i\rangle f_i^\dagger f_j - \langle f_i^\dagger f_j\rangle \langle b_j\rangle \langle b_i\rangle), \quad (3)$$

and the hamiltonian is approximated by

$$H_{MF} = H_0 + H_1 + H_2, \quad \text{where} 
H_0 = N(2\phi \psi^2 + \alpha), 
H_1 = -(\alpha + \mu) \sum_i f_i^\dagger f_i - \frac{1}{z} \psi^2 \sum_{<ij>} f_i^\dagger f_j, \quad \text{and} 
H_2 = \sum_i \left[ -\alpha b_i^\dagger b_i - \phi \psi (b_i + b_i^\dagger) \right]. \quad (4)$$

We have taken $zt = 1$ ($z$ is the coordination number of the lattice), and introduced the ground-state expectation values

$$\phi = \langle f_i^\dagger f_j\rangle, \quad \psi = \langle b_i\rangle = \langle b_i^\dagger\rangle. \quad (5)$$

We assume $\phi$ and $\psi$ to be real and homogeneous. We consider $\psi$ to be the boson superfluid amplitude [32–34] and $\phi$ to be fermion hopping amplitude. It can be observed from the expression for $H_1$ in equation (4) that when $\psi = 0$, the fermion hopping term vanishes, so $\phi = 0$. This indicates that when there is a superfluid transition in the Bose sector, there is an accompanying metal-insulator transition in the Fermi sector, resulting in the two transitions being always coupled. We have dropped the $U$-term: the hardcore boson limit $U \to \infty$ is incorporated by taking the single-site boson occupation number basis $\{|0\rangle, |1\rangle\}$ for diagonalizing the single-site $2 \times 2$ matrix

$$h_2 = \begin{bmatrix} 0 & -\phi \psi \\ -\phi \psi & -\alpha \end{bmatrix} \quad (6)$$

of $H_2/N$, with eigenvalues

$$\lambda_{\pm} = \frac{1}{2} [-\alpha \pm R], \quad \text{where} \ R = \sqrt{\alpha^2 + 4\phi^2 \psi^2}. \quad (7)$$

To solve the fermion sector hamiltonian $H_1$, we move over to $k$-space using the Fourier transform $f_i = N^{-1/2} \sum_k e^{ik \cdot r} f_k$, so that

$$H_1 = \sum_k (\varepsilon_k - \mu) f_k^\dagger f_k, \quad (8)$$

where

$$\varepsilon_k = -\alpha - \psi^2 \gamma_k \quad \text{and} \quad \gamma_k = 2(\cos k_x + \cos k_y)/z. \quad (9)$$

The zero-temperature free energy per lattice site $F = H_0/N + \langle H_1\rangle/N + \lambda_-$ is now

$$F = 2\phi \psi^2 + \frac{1}{2}(\alpha - R) + \frac{1}{N} \sum_k (\varepsilon_k - \mu) (f_k^\dagger f_k). \quad (10)$$

We observe that $\sum_k (f_k^\dagger f_k) = \rho_F$. Using the definition of $\phi$ in (5) and going over to $k$-space, we get

$$\phi = \frac{1}{Nz} \sum_{<ij>} (f_i^\dagger f_j) = \frac{1}{N} \sum_k \varepsilon_k (f_k^\dagger f_k), \quad (11)$$

so that

$$F = \frac{1}{2}(\alpha - R) + \phi \psi^2 - (\mu + \alpha)\rho_F. \quad (12)$$

Introducing the Fermi density of states

$$\rho(E) = \frac{1}{N} \sum_k \delta(E - \varepsilon_k), \quad (13)$$

we can write

$$\phi = -\frac{1}{\psi^2} \int_{E_0}^\mu dE \frac{\alpha + E}{E} \rho(E), \quad (14)$$

where $\mu$ is chosen such that the fermion filling fraction

$$\rho_F = \int_{E_0}^\mu dE \rho(E) \quad (15)$$

has a desired value. Here, $E_0 = -\alpha - \psi^2$ is the minimum value of fermion energy. To calculate the density of states [13], we convert the $k$-sum into an integral according to $\langle 1/N \rangle \sum_k \to (1/4\pi^2) \int d\mathbf{k}$. Since $\varepsilon_{-\mathbf{k}} = \varepsilon_{\mathbf{k}}$, the $k$-space
The Fermi band is 2\(\psi^2\), and therefore varies as the Fermi level (i.e. Fermi filling fraction) changes.

FIG. 2: Plots of (a) the Fermi band dispersion \(E_\mathbf{k}\) in the direction \(\Gamma X M T\) of the first Brillouin zone of the two-dimensional square lattice, and (b) the Fermi density of states \(\rho(E)\) at an arbitrary value of \(\rho_F\) in the metallic phase. The two plots share a common energy axis (ordinate). Also marked is the Fermi energy \(\mu\) at \(\rho_F\) as a horizontal line between energies \(-\alpha - \psi^2\) and \(-\alpha + \psi^2\). It can be seen that the width of the Fermi band is 2\(\psi^2\), and therefore varies as the Fermi level (i.e. Fermi filling fraction) changes.

Numerically, we find that at \(\rho_F = \rho_c \simeq 0.3\) there is a coupled transition from an insulating normal Bose gas to a metallic superfluid, with discontinuous changes in \(\psi\) and \(\phi\). \(F_0\) is continuous with a derivative discontinuity, signifying a first-order transition. Fig.1(a) shows plots of \(\psi\), \(\phi\) and Fig.1(b) shows plots of \(F_0\), \(\mu\) as \(\rho_F\) is varied. In Fig.1(c), we show a plot of the bulk modulus \(\kappa\) as \(\rho_F\) is varied. The bulk modulus has a cusp-like behavior with a value \(\phi/R = 0\) and \(\partial F/\partial \alpha = (1/2)[(1 - 2\rho_F) - \alpha/R] = 0\). We obtain two solutions for \(\psi\), namely \(\psi = 0\) (disordered, or normal Bose phase) and \(\phi = (1 - 2\rho_F)R\). We can write this as \(\alpha^2(1 - (1 - 2\rho_F)^2) = 4\phi^2\psi^2(1 - 2\rho_F)^2\), so \(\alpha = 0\), \(R = 0\), and the minimum free energy \(F_0 = 0\) in the disordered phase; in the ordered phase, \(\alpha = (1 - 2\rho_F)\phi\), \(\psi^2 = \rho_F(1 - \rho_F)\), and \(F_0 = \Delta\). Here \(\Delta = \rho_F^2[-\phi + u_F(\rho_F - 1)]\) is the minimum free energy of the ordered phase. Since \(F_0 = 0\) in the disordered phase, we can interpret \(\Delta\) as energy cost of creating superfluidity. This becomes positive for \(\rho_F < \rho_c\), a certain critical Fermi filling fraction less than 1/2 where \(u_F < 0\), as discussed in more detail (Fig. S1) in the supplementary information (SI) [39]. In the Bose-dominated regime (small \(\rho_F\)), the system therefore prefers the phase with \(\psi = 0\). This is unlike the bosonic Hubbard model [32–34,41], where the system is a superfluid for \(0 < \rho_B < 1\) in the hardcore \((U \rightarrow \infty)\) limit. Simultaneously, for \(\rho_F < \rho_c\), the Fermi sector shows an insulating phase, pointing to the important role of the coupling between Fermi and Bose sectors mediated by composite hopping. We note here that a zero-temperature insulating state with Cooper pairs has indeed been observed in amorphous Bismuth films [40].

FIG. 1: Plots of (a) \(\psi\) and \(\phi\), (b) \(F_0\) and \(\mu\), and (c) \(\kappa\) as functions of \(\rho_F\). At \(\rho_F \simeq 0.3\) there are coupled first-order transition with jumps in both \(\psi\) and \(\phi\); \(\mu\) and \(\partial F/\partial \psi\)-derivative of \(F_0\) are also discontinuous. For \(\rho_F > 0.81\), \(\mu\) and \(F_0\) decrease with \(\rho_F\), resulting in negative bulk modulus \(\kappa\), as shown in (c).

The integral is four times the integral over the first quadrant of the Brillouin zone, and so we have

\[
\rho(E) = \frac{2}{\pi^2} \int_0^\pi \frac{dk_x}{\sqrt{1 - (2u + \cos k_x)^2}}.
\]

(16)

The integral over \(k_y\) can be easily evaluated, and we get

\[
\rho(E) = \frac{2}{\pi^2} \frac{\alpha + E}{\psi^2}, \text{ where}
\]

\[
f(u) = \int_0^\pi \frac{dk_x}{\sqrt{1 - (2u + \cos k_x)^2}}.
\]

(17)

We can readily see that the function \(f(u)\) is real only when \(-1 \leq u \leq 1\), and is non-negative. Therefore we have the inequality \(-\alpha - \psi^2 \leq E \leq -\alpha + \psi^2\) for the fermion energy \(E\). The Fermi band width is therefore 2\(\psi^2\). We can also see that \(f(0) \rightarrow \infty\), and this is the van Hove singularity at \(\rho_F = 1/2\). We substitute the above expression for \(\rho(E)\) in to equations [14] and [15] and transform the integrals to obtain

\[
\rho_F = \frac{2}{\pi^2} \int_{-1}^{u_F} f(u)du, \quad \phi = -\frac{2}{\pi^2} \int_{-1}^{u_F} uf(u)du,
\]

(18)

where \(u_F = (\alpha + \mu)/\psi^2\). For a given \((\mu, T)\), we determine \(\psi\) and \(\alpha\) by simultaneously solving \(\partial F/\partial \psi = 2\psi\phi(1 - \phi/R) = 0\) and \(\partial F/\partial \alpha = (1/2)[(1 - 2\rho_F) - \alpha/R] = 0\). We obtain two solutions for \(\psi\), namely \(\psi = 0\) (disordered, or normal Bose phase) and \(\phi = (1 - 2\rho_F)R\). We can write this as \(\alpha^2(1 - (1 - 2\rho_F)^2) = 4\phi^2\psi^2(1 - 2\rho_F)^2\), so \(\alpha = 0\), \(R = 0\), and the minimum free energy \(F_0 = 0\) in the disordered phase; in the ordered phase, \(\alpha = (1 - 2\rho_F)\phi\), \(\psi^2 = \rho_F(1 - \rho_F)\), and \(F_0 = \Delta\). Here \(\Delta = \rho_F^2[-\phi + u_F(\rho_F - 1)]\) is the minimum free energy of the ordered phase. Since \(F_0 = 0\) in the disordered phase, we can interpret \(\Delta\) as energy cost of creating superfluidity. This becomes positive for \(\rho_F < \rho_c\), a certain critical Fermi filling fraction less than 1/2 where \(u_F < 0\), as discussed in more detail (Fig. S1) in the supplementary information (SI) [39]. In the Bose-dominated regime (small \(\rho_F\)), the system therefore prefers the phase with \(\psi = 0\). This is unlike the bosonic Hubbard model [32–34,41], where the system is a superfluid for \(0 < \rho_B < 1\) in the hardcore \((U \rightarrow \infty)\) limit. Simultaneously, for \(\rho_F < \rho_c\), the Fermi sector shows an insulating phase, pointing to the important role of the coupling between Fermi and Bose sectors mediated by composite hopping. We note here that a zero-temperature insulating state with Cooper pairs has indeed been observed in amorphous Bismuth films [40].
of $2\phi$ at $\rho_F = 1/2$, where the function $f(u)$ has a van Hove singularity. It can also be seen that $\kappa$ vanishes for $\rho_F = \rho_\kappa \approx 0.81$, becoming negative thereafter and approaching $-2$ at $\rho_F = 1$. This can be explained from the decreasing nature of $\mu(\rho_F)$ for $\rho_\kappa < \rho_F < 1$. This behavior of $\mu$ is determined by the filling constraint $[2]$ that results in an increasing function $\alpha(\rho_F) = (1-2\rho_F)\phi$. Very interestingly, the effective mass of fermions shows a minimum at $\rho_F = \rho_\kappa \approx 0.81$, followed by a systematic increase in the effective mass for $\rho_F > \rho_\kappa$, culminating in a divergence at $\rho_F = 1.0$ as discussed in Fig. S2. Furthermore, a negative value of $\kappa$ also corresponds to a negative compressibility of the fermions, which has been observed in two-dimensional electron gases [12] and materials with strong spin-orbit coupling [13, 44].

Fig. 3 shows plots of Fermi band dispersion $\epsilon_k$ and density of states $\rho(E)$ at an arbitrary value of $\rho_F$. The Fermi band width is $2\psi^2$, completely determined by the superfluid density. Also marked is the location of the Fermi energy $E$ as a horizontal line. We can see that $\rho(E)$ has a cusp-like singularity corresponding to energy where $\nabla_k \epsilon_k$ vanishes, and this is evidently a van Hove singularity. This singularity occurs at the Fermi energy at $\rho_F = 1/2$, and this is where the superfluid amplitude has a maximum, as can be seen in Fig. 1(a). The van Hove singularity is an important feature of the electronic structure of the high-$T_c$ cuprates [15, 49].

The Fermi surface is determined by the equation $\epsilon_k = \mu$, that simplifies to $\gamma_k = -u_F$. Fig. 3 shows plots of Fermi surface in the first Brillouin zone at five different values of $\rho_F$, namely 0.35, 1/2, 0.70, 0.81, 0.95, in the metallic phase. It can be seen that as a function of filling, the nature of carriers changes from particle-like for $\rho_F < 1/2$ (convex surface at $\rho_F = 0.35$) to hole-like for $\rho_F > 1/2$ (concave surfaces at $\rho_F = 0.70, 0.81, 0.95$), with a flat surface at $\rho_F = 1/2$. This behavior is qualitatively similar to that of a tight-binding model.

What is unusual, and distinguishes our model from the tight-binding model, is that the fermion bandwidth $2\psi^2$ changes as the chemical potential $\mu$ changes, as shown in the plots of figures 1(a), 1(b) and S3 [39].

At the van Hove point $\rho_F = 1/2$, $F_0 \approx 0.05 \, \text{zt}$ can be taken to be a reasonable approximation of $T_c$, the Bose-Einstein condensation temperature. To estimate this, we consider a situation with two neighboring sites on a lattice, one with a single electron with spin orientation $S_z = +1/2$ or $-1/2$, and the other with a pair of electrons, one with $S_z = 1/2$ and the other, $S_z = -1/2$; such a pair can be treated as a boson [24, 31]. The hopping of one of the electrons of the pair to the singly-occupied site in this situation is the same as composite hopping in model $[1]$. This could be realized in a strongly-correlated narrow single-band system above half filling, in which hopping strength is typically $\sim 0.5eV$, which would make the BEC transition temperature in our model several hundred kelvins. For simplicity we have ignored fermion spin in our model, and plan to include it in the near future.

In conclusion, we have presented a model of FBM with a hopping mechanism that exhibits several unusual properties at zero temperature. In the Bose-dominated regime, the model is in an insulating normal phase: the Fermi sector is insulating, while the Bose sector is a normal gas. As the Fermi filling fraction is increased, the model has coupled first-order transitions at $\rho_F \approx 0.3$, where superfluid amplitude $\psi$ and fermion hopping amplitude $\phi$ jump to finite nonzero values. For $\rho_F > 0.3$, the system is a metallic superfluid: the Fermi sector is metallic, while the Bose sector is a superfluid, with maximum values of $\psi, \phi$ at the van Hove singularity point $\rho_F = 1/2$ in the density of states. The bulk modulus shows a cup-like minimum here, becoming negative for $\rho_F > 0.81$. The fermion band width varies with the chemical potential $\mu$ with a maximum at $\rho_F = 1/2$, the van Hove point. And finally, our estimate for the BEC transition temperature is several hundred kelvins.

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[39] Supplementary information discusses additional details of the difference in free energies of the ordered and disordered states, the effective mass as a function of $\rho_F$, and fermionic band dispersions for representative values of $\rho_F$ corresponding to particle and hole Fermi surfaces.

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FIG. S1: Plot of $\Delta$, the energy cost of creating the superfluid phase, as a function of $\rho_F$. It can be seen that this energy cost is positive, and hence the Bose sector is normal for $0 < \rho_F < 0.3$.

Supplementary Information for the manuscript entitled “Coupled First-Order Transitions In A Fermi-Bose Mixture”.

In the manuscript, we introduced the quantity $\Delta$ (see the discussion following equation (18)), the minimum free energy of the superfluid ordered phase which is also the energy cost of creating a superfluid. Fig. S1 shows plots of minimum free energy $F_0$ in the ordered (blue) and disordered (red) phases as a function of $\rho_F$, the Fermi filling fraction. It is clear that the quantity $\Delta$ is positive for $0 < \rho_F < 0.3$, indicating that the disordered phase has a lower energy than the ordered phase. Thus, the Bose sector does not show superfluidity for $0 < \rho_F < 0.3$. And as discussed in the main text, this also leads to an insulating ground state for the Fermi sector.

Fig. S2 shows, in panel (a), the behavior of the second-derivative of $\varepsilon_k$ with respect to $k$ at Fermi energy (equation (9)), that becomes $-u_F\psi^2 \equiv -(\mu + \alpha)$ upon simplification. The panels (b) and (c) show the behavior of the inverse of this second derivative, which is the Fermi effective mass $m_e$. The effective mass changes sign from particle like ($\rho_F < 1/2$) to hole like ($\rho_F > 1/2$), and has singularities at $\rho_F = 1/2$ (the van Hove point where $u_F = 0$) and $\rho_F = 1$ (where $\psi = 0$). More interestingly, the second-derivative of $\varepsilon_k$ with respect to $k$ shows a minimum at $\rho_F = \rho_\kappa \approx 0.81$, which also corresponds to a minimum of the hole effective mass. This is followed by a systematic increase in the effective mass for $\rho_F > \rho_\kappa$, culminating in a divergence at $\rho_F = 1.0$.

In Fig. S3, we show the band dispersions for representative values of $\rho_F = 0.35, 1/2, 0.7, 0.81$ and 0.95. It is observed that the bandwidth is maximum at $\rho_F = 1/2$, (which corresponds to the case of the van Hove singularity at the Fermi energy), and decreases for values below and above $\rho_F = 1/2$. It is also clear that the band dispersions and hence the Fermi surface (see Fig. 3 of main paper) for $\rho_F = 0.35$ is particle-like and centered.

FIG. S2: Panel (a) shows the second-derivative of $\varepsilon_k$ with respect to $k$ (the reciprocal of effective mass) for $0 \leq \rho_F \leq 1$. Panels (b) and (c) show plots of the effective mass for $0.3 \leq \rho_F \leq 1$ with two different vertical scales to highlight its behavior near and away from the singularities at $\rho_F = 1/2$, 1, respectively. In panel (a), the minimum is at $\rho_\kappa \approx 0.84$; this is slightly higher than where the maximum is ($\rho_F \approx 0.81$) in the chemical potential in Fig 1(b) of main paper.

FIG. S3: Plot of band dispersions for representative values of $\rho_F = 0.35, 1/2, 0.7, 0.81$ and 0.95, corresponding to the particle and hole Fermi surfaces shown in Fig 3 of the main paper.
at the Γ-point, while for $\rho_F = 0.7, 0.81$ and 0.95, they are hole-like and centered at the M-point in the Brillouin zone.