Coherent Electron Dynamics in Thermal Lattice Vibrations

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(Dated: March 1, 2022)

We develop a coherent state description of lattice vibrations to describe their interactions with electrons. We construct the effective quasi-classical field of the interaction, called the deformation potential, and study the dynamics of an electron in this field nonperturbatively. The electron coherence is preserved well beyond a single electron scattering event. Counting the number of phonons in each vibrational mode becomes unnecessary. This is in contrast to the conventional Fock state description of lattice vibrations where an electron scattering event requires phonon creation or annihilation within the first-order perturbation theory, and multiple scatterings are treated as an incoherent and uncorrelated succession of the first-order scattering events through Boltzmann transport theory. Here, we first show the consistency of the coherent state picture with the conventional Fock state picture and then go beyond by revealing new aspects that the conventional theory could not explain. In particular, we observe electron coherence effects such as localization even at high temperatures, and density of states exhibiting Lifshitz tails and pseudogaps. Coherent electron-lattice vibration dynamics may shed light on the unexplained phenomena in strange metals such as the violation of the Mott-Ioffe-Regel limit, displaced Drude peak, existence of pseudogaps, and universal linear temperature dependence of resistivity.

I. INTRODUCTION

Crystal lattice vibrations had initially been treated essentially as a classical field, but in the first papers one phonon perturbation theory was adopted [1] [2]. Since the introduction of the second quantization, the lattice vibrations have been treated as a quantum field in Fock state picture. In this conventional description, the particle (phonon) aspect of lattice vibrations gets the most attention by design, and one rarely if ever thinks of the lattice vibrations as a classical field.

There is a viable alternative to the Fock state description, just as in quantum optics: coherent states are equivalent yet permit the construction of the quasi-classical field from the quantum field of lattice vibrations. The wave aspect of lattice vibrations is thus emphasized, providing a different perspective from the usual Fock state picture. Although it is common in quantum optics to use coherent states to describe quantized electromagnetic wave [3] [4], coherent states have rarely been used in condensed matter physics to describe quantized lattice vibrations.

In the conventional Fock state description, the interaction of an electron with lattice vibrations requires a phonon creation or annihilation within the first-order perturbation theory. Higher order interactions are approximated as an incoherent and uncorrelated chain of the first order events through Boltzmann transport theory [5] [8]. In this way, any electron coherence lasting from one collision to the next has been neglected.

Given that a phonon bath has changed in the host lattice, it might seem reasonable to neglect coherence, by the usual bath-induced decoherence arguments. However, in the quantum optical analog, this argument would be equivalent to saying that electrons cannot behave coherently in a strong electromagnetic field, which is of course not true. Note there are two different meanings of the term coherence we refer to; First, the electron coherence preserved over multiple scatterings, and second, the coherence of lattice vibrations described by coherent states.

The conventional Bloch-Grüneisen theory [9] [10] employing the Fock states picture describes the temperature dependence of electrical resistivity of most metals by taking the scattering of electrons from acoustic phonons into account. However, despite the success of the theory, there are major phenomena where the conventional methods seem to fail short, such as the mystifying superlinear temperature dependence of resistivity and universal scattering rate \( \tau = \hbar/k_BT \) in strange metals [11] [10]. The new perspective in this work, using a coherent state description of lattice vibrations, may shed light on these unexplained phenomena. We address the optimism we have in a speculative section at the end. We emphasize that we do not claim here to have “solved” the strange metal problem.

In the coherent state representation of the lattice vibrations, we lose both the ability and the need to count phonons. This is replaced by information about the phase and amplitude of each vibrational normal mode,
leaving the occupation numbers uncertain. Here, we explore the overlooked part of the wave-particle duality for lattices, considering lattice vibrations to be waves, instead of particles (phonons). We will refrain from using a word phonon and instead use lattice vibrations if possible to emphasize the wave nature. A phonon, after all, is a single, countable quantum, a particle like a photon.

We derive the palpable quasi-classical field, called the deformation potential, from the quantum field for the interaction of an electron with lattice vibrations within the coherent state representation. The deformation potential is schematically shown in Fig. 1. The interactions of an electron with this field are quasi-elastic and mostly remain coherent. Such electron coherence is absent in the conventional theories of electron-phonon interaction such as the Bloch-Grüneisen theory. Below, we do find agreement with the conventional theory whenever electron coherence is not important. The present work is therefore viewed as an extension of the current theory into the coherent regime, agreeing with the conventional approaches in the normal regimes. The electron coherence shows interesting new physics such as transient localization, even at high temperatures, and existence of Lifshitz tails and pseudogaps in density of states.

The article is organized as follows. In Sec. II we provide a historical background indicating the explicit and implicit use of the coherent state description of the lattice vibrations and electromagnetic waves in literature. In Sec. III we introduce the definition and properties of a coherent state, and then consider its application to the lattice vibrations by discussing its advantages over a Fock state. In Sec. IV we derive the explicit form of the quasi-classical field of the deformation potential and discuss its properties. In Sec. V we employ the deformation potential as a palpable non-perturbative internal field in the Hamiltonian of the system, and compare the coherent state and Fock state pictures. In Sec. VI and VII we perform full quantum calculations using the split operator method. We also implemented semiclassical ray trajectory calculations in Appendix C. There are well justified in some but certainly not all regimes of temperature and doping.

In Sec. VI we construct a temperature-Fermi momentum phase diagram obtained from our coherent state-quantum electron wavepacket numerical results. We go beyond recovering the conventional theory in Sec. VII demonstrating the existence and consequence of electron coherence and multiple scattering effects which were neglected before. In particular, we show that electrons “attempt” to localize in a short time, causing density of states exhibit Lifshitz tails and pseudogaps. The deformation potential forms exactly the kind of “slow moving Boson field” needed to explain the anomalous infrared Drude peak [17]. We discuss the possible implications of our findings in Sec. VIII and finally conclude in Sec. IX.

II. HISTORICAL BACKGROUND

The concept of what we now refer to as the coherent state of a harmonic oscillator was introduced by Erwin Schrödinger in 1926. Employing his time dependent equation, he showed that a displaced ground state oscillates without changing shape, with the mean position and mean momentum obeying classical equations of motion [18]. The extension of this result to many oscillators, including harmonic solids, is direct and straightforward [19]. This shows that any classical behavior like sound propagating through a harmonic lattice has an exact quantum analog within a coherent state representation.

Coherent states appeared in a different context in 1954, beginning with Hanbury Brown and Twiss’s [20, 21] interferometric measurement of apparent stellar diameters using two telescope mirrors spaced a variable distance apart. The field arriving from a distant star is extremely weak and presumably incoherent, so that arriving quanta (particle picture) at distant detectors were expected to be uncorrelated. Instead, Hanbury Brown and Twiss found the signal to be correlated, like advancing waves would be at nearby points on a beach. The correlation degrades as the telescopes are moved farther apart, and the decorrelation distance reveals the apparent diameter of the distant star. The implication that such weak light from an incoherent source arrived as waves did not receive a warm welcome, well after the discovery of the photoelectric effect. Eventually, however, the battle of wave vs. particle paradigms regarding the Hanbury Brown and Twiss controversy initiated the unification of the two paradigms in 1963, sparking the field of quantum optics, with coherent states playing a central role [22]. Here, we develop what might be termed quantum vibronics, a unification of Fock state and coherent state pictures of lattice vibrations, and apply it to electron-lattice interactions.

Nowadays, in addition to quantum optics [23–26], coherent states play an important role, e.g., in studies of light-matter interaction in cavity quantum electrodynamics [27], quantum chaos such as scarring [28–30], novel states of quantum matter such as superconductivity or superfluidity [31, 32]. Despite the triumph of the coherent state picture in physics, its advantage in describing the dynamics of a lattice has remained elusive, with a few rare exceptions indicating the possibility of an unused asset, such as Refs. [33, 35]. In this paper, we want to amend this conceptual shortcoming.

The present work may be viewed as a recapitulation of the Hanbury Brown-Twiss story: what had always been treated as particles (phonons in Fock states picture) is sometimes better viewed as waves (coherent states picture), within the context of a unified wave-particle theory. A terahertz (THz) lattice mode has about 13 quanta at 100 K, and a gigahertz (GHz) mode has 13,000. However, no matter how few quanta occupy the modes in a Fock space, the coherent state picture is valid, although it
FIG. 1. (a) Schematic of an atomic lattice subject to acoustic deformations. Classical path of an electron subject to the resulting deformation potential is shown by blue arrow. (b) A particular realization of the coherent state lattice vibrations at a certain temperature. Electron wave packet (real part shown in green and its direction denoted by dotted-black arrow) coherently propagates in a spatially continuous internal field formed by the acoustic deformations. Electrons quasi-elastically scatter (similar to impurity scattering) from the disordered landscape formed by the lattice vibrations.

may not necessarily be in the classical limit. In any case, weakly occupied modes play a minor role in electrical resistivity. We also remark that even a field equivalent to one photon arriving per second would show the wave-like Hanbury Brown-Twiss interference effect.

The traditional approach to the interaction of an electron with lattice vibrations traces back to the 1950 paper of Bardeen and Shockley [1, 2] who introduced the notion of a deformation potential experienced by electrons, resulting from the acoustic wave compression and dilation of the lattice. There was a moment when a classical field picture could have been adopted, but the deformation potential has instead ever since been employed exclusively in Fock states description with the first-order perturbation theory [36–41].

The traces of the idea of employing deformation potential as a real, non-perturbative field can be found only on dusty shelves of the literature. A prescient suggestion in this direction was made as early as in 1959 by Ted Holstein in a footnote [42], where he suggested a treatment of phonons based on the classical lattice-vibration wave packets, implying that he suspected the advantages of treating electrons as evolving non-perturbatively in a classical (not quantized) lattice field. However, the promised work never materialized [43].

Whenever lattice vibrations (such as sound waves) are treated classically, the coherent state representation is implied: the amplitude and phase of an oscillation give the coherent state, specifying the positions and momenta of all the atoms in the lattice. For example, Pippard [44] treated the ultrasound field produced by a transducer as a classical wave in order to interpret the observed rapid attenuation of ultrasound in metals. It would indeed seem strange to utilize a second quantized occupation number formalism for a classically occupied mode with billions of quanta.

In the classic solid state textbook by Ashcroft and Mermin [5], two chapters are devoted to “semiclassical” methods, by which is meant treating external fields acting on electrons in metals as classical fields, where the kinetic part of the Hamiltonian governed by the band structure. Lifshitz and Kosevich [45] took this methodology further by developing a coherent, semiclassical analysis, revealing the contribution of coherent semiclassical orbits on the Fermi surface to magnetic field oscillations, including the Shubnikov-de Haas effect [46]. It is evident that a coherent quantum treatment of the conduction electron in external (or internal as we do here) fields is necessary for interference effects like Shubnikov–de Haas. Non-equilibrium Green’s functions (NEGF) formalism also provides a solid framework for the study of quantum dynamics and coherence effects in general [47, 48]. While NEGF is used for coherence-preserving elastic scattering due to impurities, the scattering of electrons due to lattice vibrations have almost exclusively been employed as an incoherent process, unlike what we do in this paper.

Over the years, there have been other developments and suggestions related to what we propose here. For example, in his text Solid State Theory [49], Walter Harrison wrote

> Because of the low frequencies of the acoustical modes, it is possible to correctly compute their contributions to the electron scattering by conceptually freezing the atoms at their positions in the deformed crystal and computing the electron scattering associated with the corresponding distortions. Just as we calculated the scattering by defects in crystals.

(italics ours)

“Freezing” the atoms in position is very far from a Fock state. It is closer to a coherent state representation. Thus, it has been suspected for a long time that the deformation field can be taken at face value as a potential which would scatter electrons at the correct rate, acting like a sea of defects in the process. This implies that the inelastic creation or annihilation of phonons does not mean a stronger or weaker propensity to scatter compared to the elastic analog. This is also implied by the formal equivalence of the occupation number and coherent state representations [50], which is discussed further in Sec. [V].
This “elastic” program is already highly developed in the field of thermal diffuse scattering (TDS) from crystals. In one version of TDS, collimated electron pulses are sent through crystals; both Bragg and diffuse scattering result. The diffuse scattering increases with temperature, and changes with time if vibrational population evolution is occurring. The frozen lattice (adiabatic) approximation, i.e., supposing the lattice to be fixed at typical configurations as the electrons pass through, works extremely well at explaining the diffuse scattering and better, quantitatively exploiting it for the inverse scattering problem, yielding the geometry of lattice vibrational modes and vibrational energy evolution.

Nevertheless, the explicit utilization of the coherent state representation for lattice motion is uncommon in the literature. A notable exception is the 1972 paper by Noolandi and Kranendonk (see Refs. [33, 34]), “The use of coherent states in the theory of quantum crystals.” In their work, the aim was mainly to understand solid lattice vibrations. In one version of TDS, collimated electron pulses are sent through crystals; both Bragg and diffuse scattering result. The diffuse scattering increases with temperature, and changes with time if vibrational population evolution is occurring. The frozen lattice (adiabatic) approximation, i.e., supposing the lattice to be fixed at typical configurations as the electrons pass through, works extremely well at explaining the diffuse scattering and better, quantitatively exploiting it for the inverse scattering problem, yielding the geometry of lattice vibrational modes and vibrational energy evolution.

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emphasizes the particle nature of the lattice vibrations, whereas the former accentuates the wave nature. However, this wave-particle duality is normally hidden by the approximations the two limits encourage. Nonetheless, although at the most fundamental level the two pictures are equivalent, there are two clear benefits of employing the coherent state over the number state representation.

The first virtue of coherent states is that they are the closest quantum mechanical states to a classical description allowed by the uncertainty principle. This quantum-classical correspondence enables us to construct quasi-classical fields from quantum fields, and to study the boundary between the classical and quantum realms in general, reflecting Schrödinger’s original idea of coherent states [18]. In the limit of macroscopic occupation, the coherent state picture blends into the concept of a classical field with a fixed amplitude and phase. It is also as close as possible to a specification of the instantaneous positions and momenta of the atoms in the lattice. This explains why coherent states |αq,λ⟩ are referred to as quasi-classical. On the downside, because they are intrinsically in motion, like the lattice itself, the lattice coherent states ultimately demand a time dependent description of the field they generate on the electron. Today, this is not much of a barrier to implementation.

Second and more importantly, the coherent states |αq,λ⟩ are robust against the effect of the environment. In fact, these states are pointer states, i.e., they correspond to some value of a pointer in a classical measuring apparatus (see, e.g., Refs. [55-60]). In other words, the pointer in the measuring device can only have classical probability. Any coherent superposition of states |αq,λ⟩ is fragile and will rapidly decay to a classical probability distribution of different coherent states [58-62]. For example, a cat state constructed of coherent states will break down into a classical probability distribution since the external interactions easily destroy the quantum coherence of the initial state [55-60]. In a similar manner, squeezed states are also fragile against an influence of environment (see, e.g., Refs. [67-68]). In particular, in the presence of a perturbation such as dissipation, a high-number Fock state |nq,λ⟩ promptly decomposes into an incoherent linear combination of coherent states |αq,λ⟩ with different phases ϕq,λ and amplitude ~ nq,λ (see, e.g., Refs. [25, 69-71]). In this light, it is natural to describe the lattice vibrations in terms of the coherent states.

Since the vibrational normal modes are independent of one another, the entire lattice vibrations as a whole can be described with the product state of the coherent states |αq,λ⟩ of the normal modes q,λ’s, a multimode coherent state

\[ |\chi\rangle = \prod_{q,\lambda} |\alpha_{q,\lambda}\rangle, \]  

as considered in Ref. [19]. A realistic lattice is coupled to an environment which is expressible employing thermal ensembles of coherent states [72, 73]. Therefore, we consider that each mode is in thermal equilibrium with a heat bath at temperature T, and the average number of quanta of corresponding coherent states follows the Bose-Einstein statistics, i.e.,

\[ N_{q,\lambda} = \langle n_{q,\lambda}\rangle_{th} = \frac{1}{\exp(\hbar \omega_{q,\lambda} / k_B T) - 1}. \]  

The amplitudes of the modes |αq,λ⟩ are determined by taking the thermal average value in Eq. (7) for the average occupation in Eq. (5):

\[ \langle \alpha_{q,\lambda}\rangle^2 = N_{q,\lambda}. \]  

This approach of associating the thermal average value with the average occupation has been widely utilized as a natural pathway to thermalize a field, e.g., by Bardeen and Shockley for a classical field of lattice vibration [2], and by Hanbury Brown and Twiss for a classical field of electromagnetic wave [20].

In general, the coherent state |χ⟩ gives the exact quantum dynamics of the entire lattice. However, we can take a next step by following the similar road as in the theory of quantized electromagnetic fields: by merging the concepts of the quantum lattice vibration field and the (thermal) coherent states, we construct a quasi-classical lattice vibration field that yields the deformation potential.

IV. DEFORMATION POTENTIAL

Inspired by the coherent state picture of lattice vibrations described in the previous section, we introduce a new framework for the interaction of an electron with lattice vibrations. We begin with second-quantized form of lattice vibrations, then derive the deformation potential employing the thermal ensemble of coherent states.

The concept of the deformation potential was first introduced by Bardeen and Shockley for non-polar semiconductors [1, 2]. The main idea is that local electronic band energy can be used as an effective potential when the variation of the lattice distortions are sufficiently gradual. This is the case for the long-wavelength longitudinal acoustic lattice deformation which interact with electrons of thermal velocity. In this work, optical lattice deformation is not considered since its thermal population is smaller than the acoustic lattice deformation. Furthermore, it generates sudden variation of the lattice distortions inside the unit cell which can be subtle to implement within the deformation potential approach [74].

A. Derivation

In a distorted lattice, lattice deformation is characterized by a displacement field \(u(x)\) that is a displacement of an atom at a position \(x\) from its equilibrium position. The displacement field gives strain fields \(\epsilon_{ij}(x) = \frac{\partial u_j(x)}{\partial x_i}\).
where the parameter be noted that only the longitudinal \((\lambda = l)\) acoustic modes contribute to the deformation potential \((q \cdot \varepsilon_{ql} = q)\), whereas the transverse \((\lambda = t)\) acoustic modes do not \((q \cdot \varepsilon_{qt} = 0)\).

We next construct a corresponding quasi-classical field of the deformation potential \(V_D(r, t)\) by taking the expectation value of the quantum field of the deformation potential \(\hat{V}_D(r, t)\) with respect to the multimode coherent state \(|\chi\rangle\) (see Eq. 6) describing the lattice.

\[
V_D(r, t) = \langle \chi | \hat{V}_D(r, t) | \chi \rangle = -\sum_q g_q (\alpha_{ql} e^{-i\omega_{ql}t} + \alpha^*_{ql} e^{i\omega_{ql}t}) e^{iq \cdot r} \tag{14}
\]

The amplitudes of the modes \(\sim |\alpha_{ql}|\) are determined by the thermal occupations (see Eq. 6).

Now we use the Debye model that introduces linear dispersion \(\omega_{ql} = v_s |q|\) \((v_s\) is sound speed\) and Debye wavenumber (isotropic cutoff) \(q_D\). Then, the quasi-classical field of the deformation potential is written as

\[
V_D(r, t) = -\sum_{q < q_D} g_q \sqrt{N_{ql}} \cos(q \cdot r - \omega_{ql} t + \varphi_{ql}) \tag{15}
\]

where \(\varphi_{ql} = \arg(\alpha_{ql})\) is the phase of a coherent state \(|\alpha_{ql}\rangle\). Examples of this potential are given in Figs. 1, 3 and 4.

We want to emphasize two aspects regarding the derivation. First, although our deformation potential was derived from the quantized lattice vibrations, it can also be deduced from the classical lattice vibrations as shown in Appendix A. Second, the lattice model is not necessarily to be the Debye model and any appropriate dispersion relation \(\omega_{ql}\) can be used. Nevertheless, we will use the Debye model, assuming the linear dispersion \(\omega_{ql} = v_s q\).

We should also note that a very similar expression was derived in 1957 by Hanbury Brown and Twiss for the vector potential of a blackbody field \([77, 78]\). The forces acting on electrons in the blackbody field is very similar to the forces acting on electrons in the deformation potential field. However, the essential difference between these two is in the existence of the ultraviolet cutoff \(q_D\) in the deformation potential originating from the minimal lattice spacing.

### B. Properties

There are important statistical properties of the deformation potential. We treat either position \(r\), time \(t\), or phase \(\varphi_{ql}\) appearing in Eq. 15 as uniformly distributed random variables. Then, the deformation potential value \(V_D\) is a random variable normally distributed with mean \(\mu_{V_D}\) and standard deviation \(\sigma_{V_D}\) by the central limit theorem, i.e.,

\[V_D \sim \mathcal{N}(\mu_{V_D}, \sigma^2_{V_D})\]
The mean is zero $\mu_{V_D} = \langle V_D \rangle = 0$ and the standard deviation is root-mean-square of the potential values $\sigma_{V_D} = \sqrt{\langle V_D^2 \rangle} = V_{\text{rms}}$. Note the average $\langle \cdot \rangle$ can be taken over the chosen random variables; they all give the identical results as they appear in the argument of the same cosine in Eq. (15).

The potential is homogeneously random [20] in spacetime, meaning the probability distribution of $V_D$ does not depend on a position $r$ or time $t$ given that the phases $\phi_q$ are random variables. Thus, each spatio-temporal section of the potential is statistically indistinguishable from another.

The spatio-temporal autocorrelation function $C(\delta r, \delta t) = \langle V_D(r, t) V_D(r + \delta r, t + \delta t) \rangle$ gives the strength of the potential fluctuation and the decay of its spatio-temporal correlation (see more details in Appendix A). In 2D, the autocorrelation is

$$C^{(2D)}(\delta r, \delta t) = \frac{V}{(2\pi)^2} \int_0^{qD} g_q^2 N_q \pi J_0(q \delta r) \cos(v_q q \delta t) dq dq$$

(16)

The autocorrelation is significant for a spatio-temporal relation $\delta r = v_s \delta t$ corresponding to the sound wave propagation.

From the autocorrelation, we can obtain the typical energy scale of the potential fluctuation, i.e., the root mean square of the potential values $V_{\text{rms}} = \sqrt{C(0, 0)}$. Note although the electron-phonon coupling amplitude of each mode $g_q \sim 1/\sqrt{V}$ has a volume dependence, the potential fluctuation $V_{\text{rms}}$ does not. This is because the number of modes $\sim V$ cancel the volume dependence out as shown in $V g_q^2$ factor in Eq. (16).

The typical length scale of the potential is determined by its largest wavenumber components. At temperature $T$, a Bose wavenumber $q_B(T) = k_B T / \hbar v_s$ determines the effective largest wavenumber from the thermal occupation. The modes below the Bose wavenumber ($q < q_B(T)$) are thermally active while the modes above the Bose wavenumber ($q > q_B(T)$) are effectively frozen out; the Bose wavenumber $q_B(T)$ acts as a soft thermal cutoff. The actual effective thermal cutoff is given roughly by $5q_B(T)$ as the factor $g_q \sqrt{N_q}$ in Eq. (15) becomes negligible for $q \gtrsim 5q_B(T)$. Thus, the effective wavenumber cutoff is the minimum of $5q_B(T)$ and $q_D$, i.e., $q_{\text{eff}}(T) = \min\{5q_B(T), q_D\}$, which determines the length scale of the potential.

For $T < 0.2 T_D$, the potential effectively does not “notice” the existence of the Debye cutoff $q_D$ since the thermal cutoff $5q_B(T)$ comes first, i.e., $q_{\text{eff}}(T) = 5q_B(T)$. Fig. 3 shows the deformation potential at the two different temperatures both below $0.2 T_D$. In this temperature range, as the temperature $T$ increases, the effective largest wavenumber $q_{\text{eff}}(T) = 5q_B(T)$ increases, thereby shorter length scale emerges. In addition, as the amplitude of each mode increases as the temperature increases, one can see the bumps and dips get higher and deeper.

Furthermore, as shown in the top panel of Fig. 4, the sizes of bumps and dips are characterized by the length scale $2\pi / 5q_B$ of the spatial autocorrelation decay. For $T > 0.2 T_D$, the potential notices the Debye cutoff $q_D$, i.e., $q_{\text{eff}}(T) = q_D$ and the relevant length scale $\sim 2\pi / q_D$ is seen in both the potential and the autocorrelation function as shown in the bottom panel of Fig. 4.

Similarly, the typical timescale of the potential change is determined by its largest frequency components. Temporal autocorrelation function $C(0, \delta t)$ gives the characteristic timescale of the change of the potential, which is given by $2\pi / 5 \omega_B$ for $T < 0.2 T_D$, and $2\pi / \omega_D$ for $T > 0.2 T_D$ where $\omega_B = v_s q_B$ and $\omega_D = v_s q_D$ (see more details in Appendix A).

C. Usage

The electronic band energy in Eq. (9) can be treated as a Hamiltonian for an electron:

$$H(\hbar k, r, t) = E_0(k) + V_D(r, t)$$

(17)

where $k$ is an electron wavevector, $E_0(k)$ is band energy of undistorted (hence periodic) lattice and $V_D(r, t)$ is the quasi-classical field of the deformation potential in Eq. (15). The dynamics of the electron under the Hamiltonian can be studied by solving the time-dependent Schrödinger equation.

We use the effective mass model $E_0(k) = \hbar^2 k^2 / 2 m^*$ where $m^*$ is an effective mass of an electron. Any initial wavefunction can be used, but the Gaussian wavepacket with an initial momentum is a reasonable choice for studying electron transport. Although any energy of conduction (valence) electron can be considered, we mostly examine electrons with Fermi energy $E_F = \hbar^2 k_F^2 / 2 m^*$, as the important carriers. Electron wavepackets with an initial momentum $\hbar k_F$ are thus investigated.

Since the Fermi velocity is far faster than the sound speed, $v_F \gg v_s$, the electron quickly enters into a new region that is uncorrelated to its original region. Then, as the potential is homogeneously random, the uncorrelated

![FIG. 3. Contour plots of the deformation potential at 20K and 30K demonstrating the opening of new vibrational modes with increasing temperature. Both the legend and the lattice length are given in arbitrary scale for illustration purposes. Identical random phases are used to generate the deformation potential for both temperatures. The bumps and dips also get higher and deeper with increasing temperature.](image-url)
new region is statistically indistinguishable from another region of the potential at another time. Thus, the electron dynamics in the deformation potential $V_D(r,t)$ can be approximated as the dynamics in frozen deformation potential $V_D(r,t=0)$ when $v_F \gg v_s$.

This picture however will to be reconsidered under the much slower, semi-localized motion induced by the deformation potential that we find below. Here, we use a frozen deformation potential. We have some trials with dynamic deformation potentials and do not see large effects in short times. More investigations with dynamic deformation potentials are planned.

The Drude theory of metals states that, for a metal with a carrier of an effective mass $m^*$, an absolute value of charge $e$, and carrier density $n$, electrical resistivity $\rho$ is determined by the momentum relaxation time $\tau$ through the relation $\rho = m^*/n e^2 \tau$. We focus on the inverse momentum relaxation time $1/\tau$ in place of resistivity $\rho$.

**V. COMPARISON OF COHERENT AND FOCK STATE PICTURES**

We compare here the Fock state second-quantized and coherent state formulations of the deformation potential in Eq. (12) and the coherent state. In the perturbative Fock state picture, phonon creation/annihilation accompanies electron-phonon interaction. In the coherent state description, this issue is different. The quantum field in Eq. (12) naturally reduces to the quasi-classical field in Eq. (8). Then, one no longer counts the number of phonons in lattice vibrations and electron can be scattered by the potential without explicit phonon creation/annihilation, just as an impurity scattering. However clearly electron-phonon energy exchange occurs, and a complete understanding must include its effects. For example the energy relaxation and thermalization must depend on it. We reserve this for future work and operate for now in the classical field limit well known in quantum optics.

The coherent state picture used here is not intrinsically electron-lattice energy exchange, just as the Fock state picture is not intrinsically incoherent and perturbative.

**A. Perturbation theory and reciprocal space diagram**

Here we use perturbation theory to study the difference between the coherent and Fock states descriptions. For simplicity, we do not deal with Fermi statistics for now. We encourage readers to look at Appendix B for details of the calculations.

First, we look into coherent state description. For an electron in the deformation potential $V_D(r)$, the inverse of the momentum relaxation time $1/\tau$ for an initial state $|k\rangle$ is determined by the sum of the transition rates $\Gamma_{k\rightarrow k+q}$ from initial state $|k\rangle$ to any final state $|k+q\rangle$, weighted by the factor $(1 - \cos \theta_{k,k+q})$ which quantifies how much the momentum autocorrelation decreases for the scattering angle $\theta_{k,k+q}$:

$$\frac{1}{\tau_{el}} = \sum_{k'} \Gamma_{k\rightarrow k'} (1 - \cos \theta_{k,k+q})$$  \hspace{1cm} (18)

where the transition rates are given by Fermi’s golden rule

$$\Gamma_{k\rightarrow k+q} = \frac{2\pi}{\hbar} \left| g_q \right|^2 N_q \delta(\varepsilon(k+q) - \varepsilon(k))$$

and $g_q = g \Theta(q_D - q)$ is electron-phonon coupling strength including the Debye cutoff $q_D$. The subscript
creation processes using Fermi’s golden rule are

\[ \frac{1}{\tau_{in}} = \sum_q \left[ \Gamma_{k \rightarrow k+q}^{(1)} (1 - \cos \theta_{k,k+q}) + \Gamma_{k \rightarrow k-q}^{(2)} (1 - \cos \theta_{k,k-q}) \right] \]

where the transition rates of phonon annihilation and creation processes using Fermi’s golden rule are

\[ \Gamma_{k \rightarrow k+q}^{(1)} = \frac{2\pi}{\hbar} |g_q^<|^2 N_q \delta(\varepsilon(k+q) - \varepsilon(k) - \hbar \omega_q) \]

\[ \Gamma_{k \rightarrow k-q}^{(2)} = \frac{2\pi}{\hbar} |g_q^<|^2 (N_q + 1) \delta(\varepsilon(k-q) - \varepsilon(k) + \hbar \omega_q) \]

respectively. Note inelastic scattering \( \varepsilon(k \pm q) = \varepsilon(k) \pm \hbar \omega_q \) naturally came out due to the creation and annihilation operators in Eq. \((12)\). This is in contrast to the perturbation theory in coherent state picture in Eq. \((18)\) where elastic scattering naturally came out.

In the quasielastic approximation \( \hbar \omega_q \ll \varepsilon(k') \), \( \varepsilon(k) \), the inelastic scattering matrix element \( |g_q^<|^2 \delta(\varepsilon(k+q) - \varepsilon(k) - \hbar \omega_q) \) does not differ much from the elastic scattering matrix element \( |g_q^<|^2 \delta(\varepsilon(k\pm q) - \varepsilon(k)) \). Thus, without considering Fermi statistics, the two pictures give almost the same momentum relaxation time (see more details in Appendix \(3\)).

In both pictures, the calculation can be easily demonstrated with the reciprocal space diagram for the scattering shown in Fig. \(5\). The contour of equal electronic energy is drawn as a blue circle with a radius \( k_F \) varying only about the horizontal axis. Fourier transform of the deformation potential is shown as a yellow disk depending only on temperature \( T \), the vertical axis. The radius of the yellow disk is determined by the Bose wavenumber \( q_B(T) \) roughly up to which normal modes are thermally occupied. Also, the thickness of yellow disk reflects the occupation number of each mode increasing with temperature. In addition, a dashed gray circle shows the Debye cutoff \( q_D \). Then, the possible scattering processes appear at the intersections of the blue circle and yellow disk.

The critical temperature separating low and high temperature behaviors are different in the following two regimes:

(i) \( 2k_F > q_D \) (e.g., typical metals). The maximal scattering wavenumber is given by Debye wavenumber \( q_D \), and the critical temperature is given by the corresponding Debye temperature \( T_D = \hbar \nu_s q_D / k_B \).

(ii) \( 2k_F < q_D \) (e.g., semimetals). The maximal scattering wavenumber is given by twice the Fermi wavenumber \( 2k_F \) (backscattering), and the critical temperature is given by the corresponding Bloch-Grüneisen temperature \( T_{BG} = \hbar \nu_s 2k_F / k_B \). Although there exist shorter wavelength modes \( q > 2k_F \), they do not contribute to scattering the electron as there is no energy conserving transition for them. We say the electron is “transparent” to the shorter wavelength modes \( q > 2k_F \).

We define the regime-independent parameters: the maximal scattering wavenumber \( q_{max} = \min\{q_D, 2k_F\} \) and the corresponding critical temperature \( T_c = \hbar \nu_s q_{max} / k_B = \min\{T_D, T_{BG}\} \). The critical temperature divides low and high temperature behaviors:

(i) For low temperature limit \( T \ll T_c \), the number of thermally activated modes rises as \( q_B(T) \sim T \) in 2D \( ((q_B(T))^2 \sim T^2) \) in 3D), the square of the matrix element increases as \( |g_q|^2 \sim T \), and the geometric factor by \( 1 - \cos \theta \sim T^2 \), giving \( 1/\tau \sim T^4 \) in 2D \( (\sim T^6 \) in 3D).

(ii) For high temperature limit \( T \gg T_c \), only the square of the matrix element increases with temperature \( |g_q|^2 \sim T \), so resistivity goes as \( 1/\tau \sim T \).

B. Comparison considering Fermi statistics

In the previous section, we showed the coherent and Fock state pictures give almost the same inverse momen-
tum relaxation time if the Fermi statistics is not considered. However, the two approaches give slightly different results if Fermi statistics is considered (see details in Appendix B). Taking Fermi statistics into account, the inverse momentum relaxation time for the deformation potential in 2D in the two pictures are

$$\left\langle \frac{1}{\tau_{cl}} \right\rangle = \frac{m^*}{2\pi\hbar^3 k_F^2} \int_{q=0}^{q_{max}} \frac{dq q^2}{\sqrt{1 - (q/2k_F)^2}} \frac{E^2 \hbar q}{\rho_m v_s} N_{ql}$$

(20)

$$\left\langle \frac{1}{\tau_{1n}} \right\rangle \approx \frac{m^*}{2\pi\hbar^3 k_F^2} \int_{q=0}^{q_{max}} \frac{dq q^2}{\sqrt{1 - (q/2k_F)^2}} \frac{E^2 \hbar q}{\rho_m v_s} \times N_{ql}(N_{ql} + 1)\beta \hbar \omega_{ql}$$

(21)

Both give correct low and high temperature dependence, as shown in Fig. 6. The only difference is that the inelastic scattering result has additional factor $(N_{ql} + 1)\beta \hbar \omega_{ql} \geq 1$ compared to the elastic scattering result, making inelastic scattering stronger than the elastic only if Fermi statistics is considered. In the high temperature limit where all the phonon energies are small compared to thermal energy, the factor becomes unity $\lim_{\beta \hbar \omega_{ql} \to 0} (N_{ql} + 1)\beta \hbar \omega_{ql} = 1$, so there is no difference between the two pictures in high temperature limit within the perturbation theory.

A distinguishable difference is in the low temperature part. Both give correct temperature dependence, but their proportionality constants differ: $\left\langle 1/\tau_{1n} \right\rangle = 4 \left\langle 1/\tau_{cl} \right\rangle \sim T^4$ for $T \ll T_c$ (ln 3D, $\left\langle 1/\tau_{1n} \right\rangle = 5 \left\langle 1/\tau_{cl} \right\rangle \sim T^5$ for $T \ll T_c$). Such difference could be significant, but it is hard to know which fits experimental data better. As long as both give the correct temperature dependence in low and high temperature limits, the parameter (in this case deformation potential constant) can be adjusted to fit the experimental data better. As the deformation potential constant value varies among the literature, it can be thought as a “free parameter” upto some extent \cite{82,85}.

VI. ELECTRON DYNAMICS WITH COHERENT STATE LATTICE VIBRATIONS

In this section, we focus on nonperturbative Schrödinger electron dynamics under the coherent state description of lattice vibrations. We use the the split operator method for electron wavepacket propagation \cite{86,88}. We launch electron wavepackets with an initial average momentum $\hbar k_F$ on the deformation potential $V_D$.

We use the results to construct a temperature-Fermi momentum phase diagram of the inverse momentum relaxation time $1/\tau$. As in the reciprocal space diagram in Fig. 7, we use dimensionless parameters $T/T_D$ and $2kF/qD$ for axes. As there are no sharp boundaries between the different behaviors; the changes as crossovers rather than phase transitions. We have following parameters qualitatively affecting the dynamics:

(i) $V_{rms}/E_F$, the ratio of the potential fluctuation $V_{rms}$ to the average kinetic energy of the wavepacket $E_F$. $V_{rms}/E_F \ll 1$ where the potential is a perturbation to the free (effective mass) electron motion. This is the regime of normal metals. $V_{rms}/E_F \gtrsim 1$ is the non-perturbative regime where the electron is strongly scattered, or even partially trapped by the potential, showing very different dynamics from the perturbed free (effective mass) electron motion.

(ii) $kF/q_{eff}(T)$ is the ratio of effective shortest wavelength $2\pi/q_{eff}(T)$ of the potential to electron wave-length $2\pi/k_F$. The classical regime is $kF/q_{eff}(T) \gg 1$ where the electron wavelength is shorter than the effective shortest length scale of the deformation potential.

The temperature-Fermi momentum phase diagram using typical metal and doped metal parameters (see Supplemental Material) is shown in Fig. 7.

The following are explanations for distinct regions with different characteristics:

(i) Region I. This is the highly nonperturbative ($V_{rms}/E_F > 0.5$) localization region. Electrons are scattered by a strong deformation potential, which would cause electrons to localize in short distances under a frozen deformation potential. However, the time depen-
FIG. 7. Temperature-Fermi momentum phase diagram from numerics. In region I, electrons are scattered by a strong deformation potential, which can cause electrons to localize under the frozen deformation potential. The region II shows perturbative and non-classical behavior such as wave interference and diffraction. The region III shows perturbative and classical behavior. The red dashed line ($V_{\text{rms}}/E_F = 0.3$) divides perturbative and non-perturbative regions. The white dashed line ($T = 0.1T_c$) divides the low ($1/\tau \sim T^4$ for $T \ll T_c$) and high ($1/\tau \sim T$ for $T \gg T_c$) temperature behaviors.

dence of the potential would presumably break the localization, causing transient localization [89–91]. This will be discussed in the next section.

(ii) Region II. This is the perturbative ($V_{\text{rms}}/E_F < 0.15$) and non-classical ($k_F < q_{\text{eff}}(T)$) region. Wave interference and diffraction are observed. There is a partial transparency of the electrons to any shorter wavelength modes ($q > 2k_F$) present in the underlying deformation potential [81] as was explained in Sec. V A.

(iii) Region III. This is the perturbative ($V_{\text{rms}}/E_F < 0.15$) and classical ($k_F \lesssim q_{\text{eff}}(T)$) region. Classical behaviors such as forward scattering and branched flow [81, 92, 93] are observed as shown in Fig. 8. Exponential decay of the average momentum of the wavepacket is observed. The momentum relaxation time was obtained using linear regression in log plot. In this region Fermi’s golden rule (Eq. (20)) works very well.

We also ran the classical simulation and checked that it gives consistent results with the quantum dynamics described above (see more details in Appendix C). As the classical dynamics cannot capture wave nature of the electron such as interference and diffraction, it is no longer valid in the non-classical regime $k_F/q_{\text{eff}}(T) \lesssim 1$. Thus, in this work, we will focus on quantum dynamics in the main text, leaving the discussion of classical dynamics to Appendix C.

VII. ELECTRON COHERENCE EFFECTS

Coherent dynamics of an electron interacting with lattice vibrations not only recover the correct temperature dependence of resistivity in metals, but also lead to new
results which the conventional formalism (incoherent and uncorrelated succession of the first order events through Boltzmann transport theory) was unable to capture. In this section, we discuss the electron coherence effects that are carried beyond the single collision events, which may have important consequences for electron transport.

A. Localization at high temperatures

In our wave packet simulations, we find electrons to be localized by the frozen deformation potential in long Fermi wavelength and high temperature regime (region I in Fig. 7). To investigate this regime further in detail, we choose strange metal parameters (see Supplemental Material), rather than the typical metal ones. In particular, we use \( 2k_F/q_D = 0.5, T/T_D = 1 \) and \( V_{\text{rms}}/E_F = 1.87 \) as our dimensionless parameters.

The result of the simulation is shown in Fig. 10. The wave packet with an initial momentum \( h k_F \) (Fig. 10(a)) is launched to the right under the deformation potential. Momentum space picture is shown in the bottom-left inset. Fig. 10(b) shows the snapshot of the wave packet after 50 fs is passed. Due to the strong scattering and interference, the wave packet is localized in real space, indicated by the dashed black circle.

We observe four different signatures of Anderson localization. (1) The exponential decay of radial probability density in Fig. 10(c). Linear wings in the log-linear plot suggests that the density profile decays exponentially from the initial launch point of the wave packet. (2) Rapid average momentum reversal in the inset of Fig. 10(d), implying the electron wave packet tries to return toward its initial launch point, which is similar to the quantum boomerang effect. (3) The decrease of mean distance in the transport direction in Fig. 10(d), indicating the exponential decay of the density profile radially in 2D space. (d) Fast saturation of the mean distance as well as a slight quantum-boomeranglike effect is shown. The inset shows the rapid decay of the average momentum to zero. After the rapid initial decay, average momentum of the wave packet oscillates around zero.

![Image](image-url)

**FIG. 10.** Localization of the wave packet at \( 2k_F/q_D = 0.5, T/T_D = 1 \) and \( V_{\text{rms}}/E_F = 1.87 \). (a) At \( t = 0 \) wave packet is launched to the right with an initial momentum \( k \). On the bottom-left momentum space picture is shown as inset. (b) Within a very short time \( t < \tau_\phi \), the wave packet is localized by the frozen deformation potential. (c) Log-linear plot of radial probability density versus position (radial distance) indicates the exponential decay of the density profile radially in 2D space. (d) Fast saturation of the mean distance as well as a slight quantum-boomeranglike effect is shown. The inset shows the rapid decay of the average momentum to zero. After the rapid initial decay, average momentum of the wave packet oscillates around zero.

B. Density of states, Lifshitz tails and pseudogaps

We have another opportunity unavailable to the Bloch-Grüneisen theory in a Fock state description, namely to accurately calculate the quantum single electron density of states as a function of energy. As we are already operating in the time domain, we can evaluate the total density of states per unit volume as a trace over coherent states \( |a\rangle \) for the electron, which are of course a complete longer times, but before fully diffusive behavior is established, the lattice dynamics can delocalize the charge carriers, a phenomenon so-called transient localization [93–95]. In the transient localization, electrons encounter time varying landscapes of disorder, which breaks the quantum interference causing localization, initiating the delocalization of electron wavefunctions [97, 98]. Due to strong scattering and transient localization effects, electron motion slows down. As a result, short-time localization as well as its breakdown at longer times may affect the transport properties in the materials showing bad/strange metal behavior.
FIG. 11. Lifshitz tail and pseudogap in a 2D density of states with a deformation potential present. The black curve is calculated from 14,400 plane waves as a basis set in a large patch of the potential. $E = 0$ is the nominal, zero Kelvin threshold. The red area is a tail extending below zero energy. If the measured threshold is used as the origin, a significant pseudogap appears at the threshold.

basis, as

$$\rho_{\text{tot}}(E) = \frac{1}{V} \text{Trace} \left[ \delta(E - H(\hat{p}, \hat{q})) \right] = \frac{1}{V} \int dt \ e^{iE t / \hbar} \frac{1}{\pi} \int d^2 \alpha |\alpha\rangle e^{-iH t / \hbar} |\alpha\rangle$$

(22)

The time-dependent state $|\alpha(t)\rangle = e^{-iH t / \hbar} |\alpha\rangle$ is precisely the workhorse for our quantum treatment of electrons. Advantages in using this form include limiting the time interval to a range commensurate with the required frequency resolution. If for example there are density of states pseudogaps on the order of $0.05 - 0.1$ eV, then we need to evaluate the coherent state autocorrelations for a time on the order of $10^{-14}$ seconds.

Oscillations in the density of states, interpreted as pseudogaps, are seen by angle-resolved photoemission spectroscopy (ARPES) spectra of strange metals. We observe similar anomalies in the density of states, which may be referred to as pseudogaps. The pseudogap is here defined as a depression in the single-particle density of states near the Fermi energy, relative to a “normal” density of states.

The roiling deformation sea causes dramatic effects on the band structure near threshold, compared to a smooth band. Some energies fall below the nominal, smooth band minimum, at any finite temperature. This causes a deficiency in the density of states above the nominal band origin, see hatched area in Fig. 11. These can be interpreted as pseudogaps, depending on where threshold is figured. This fascinating effect is related to Lifshitz tails shown in Fig. 11, a subject we are actively investigating.

VIII. DISCUSSION

The short-time localization attempt of electrons we find suggests the existence of a strongly correlated electron-lattice vibrations mix. Electrons may be confined in the slow moving potential, forming near-Anderson localized quasiparticles. These may collectively form an emergent fluid as it is suggested before in the context of strange metals for different reasons. The formation of correlated fluid would involve polaron-like lattice relaxation, which might be a precursor to full charge density wave formation that occupies a part of the doping-temperature phase diagram of strange metals. The resistivity of such a fluid might be independent of the details of the interactions.

It is worth remarking that lattice vibrations, so important to other aspects of transport in crystals, would also play an essential role in strange metal properties. Without claiming that solutions are in hand, the correlated fluid picture could have implications for each of the “big six” strange metal properties: (1) absence/displacement of the Drude peak (as would befit localized particles), (2) formation of pseudogaps (which might have a similar origin of what we observed here), (3) superconductivity (new type of correlation between electron and lattice vibrations), (4) linear T dependence of resistivity with scattering time $\tau \sim h / k_B T$ (via the breaking of transient localization), (5) bypassing the Mott-Ioffe-Regel saturation limit, and (6) A charge density wave phase (consistent with strong electron-lattice vibrations interactions in nearby regions).

Violation of Mott-Ioffe-Regel limit

At high temperatures, Mott-Ioffe-Regel phenomena center on very small mean free paths, on the order of lattice constants. This regime should be fertile territory for Anderson localization, yet the strict perturbative, incoherent models suppose localization to be moot. We do not believe localization is moot at high temperatures. It should be noted that even the failed localization attempts (due to lattice dynamics) might seriously alter the incoherent Drude-like picture of resistivity. The violation of Mott-Ioffe-Regel limit and nonsaturation of resistivity of some metals at high temperatures, for example, can be a consequence of the transient localization phenomenon, which hinders the transport.

Displaced Drude peak

In a recent paper, Fratini and Ciuchi showed that “slow Boson modes” explain the anomalous infrared displaced Drude peak behavior of the strange metals. They did not specify what these slow modes are. We believe they are very likely the deformation potential, as described here.

Linear T resistivity and universal “speed limit” relaxation time

Both of these well known mysteries of the strange met-
als seem to be consistent with our deformation sea. The arguments depend critically on electron coherence. The rough idea goes like this: Energy cannot be exchanged between different quantum degrees of freedom faster than the available energy \((k_B T)\) allows, enforced by the uncertainty principle

\[
\tau \geq \frac{\hbar}{k_B T}.
\]

According to this work, the deformation potential sea would be the agent of the exchange, and its growth in amplitude as \(T\) strongly suggests linear \(T\) resistivity, since it can be figured from energy relaxation rate.

Including back-action

These thoughts are admittedly speculative, but speculation is common currency so far in the strange metal world.

Here, our attention focuses on electron motion in a deformation field, ignoring any back-action of the electron on the field. Particularly, the local lattice response to a localized or quasi-trapped electron has not been taken into account, but one can easily imagine polaron-like scenarios.

The avenue is open to including back action, respecting the fluctuation-dissipation theorem and electron-lattice vibrations coupling as a thermalization pathway, which we plan for a future work. We suspect an absence of an infrared spectroscopic Drude peak due to the transient localization, which is another direction under consideration.

Beyond the continuum

In the present work, we have considered the lattice to be a smooth continuum. Nonetheless, it is also possible to embed the problem within a discrete model: time dependent tight binding calculation, including the effect of lattice vibrations as time dependent hopping parameters, as was done for graphene within the time-dependent Schrödinger equation with no Born-Oppenheimer approximation [53].

IX. CONCLUSION

We have introduced a coherent state description of lattice vibrations and re-cast interactions with electrons, providing a quite different paradigm for electron-phonon interactions than the conventional Fock state description. In the coherent state description, the quasi-classical field of the deformation potential acting as a non-perturbative internal field on electrons and preserving their coherence for many collisions. This is analogous to an electron subject to a classical blackbody electromagnetic radiation field; photons are not counted, and the back-action of an electron on the incident field is neglected [113]. In contrast, in the Bloch-Grüneisen theory within the Fock state description of lattice vibrations, any electron coherence effects lasting longer than a single collision time are lost, since higher order scattering is approximated as an incoherent and uncorrelated concatenation of first order scattering events through Boltzmann transport [7] [114].

We successfully performed both semiclassical (in Appendix C) and fully quantum (in the main text) analysis of the problem using ray trajectory and wave packet propagation calculations, respectively. We find an agreement with Bloch-Grüneisen theory in the weak field limit, and also go beyond by retaining the electron coherence over longer times, revealing high temperature coherence effects. For strong fields at high temperatures, the “attempted” localization introduces crucial modifications on carrier transport, which might be related to the strange metal phase. We conclude that the electrons can remain coherent in spite of conversing with huge numbers of phonons, in an analogy with electrons in an electromagnetic field.

The wave picture of the lattice vibrations introduced in this paper opens new vistas unavailable using second quantized electron-phonon perturbation theory.

The nonperturbative treatment of the electron dynamics in the deformation potential has revealed the importance of electron coherence effects such as localization, Lifshitz tails and pseudogaps in density of states. The coherent state paradigm of lattice vibrations gives a fresh perspective on important open questions in condensed matter physics, most importantly the properties of strange metals.

One goal of future work is to apply these ideas to semiconductors, which after all were the target of Bardeen’s original deformation potential work.

The semiclassical forces on conduction electrons we identify here are not conjectural; they are direct consequences of known physics. The quantum vibronics we develop in the paper is a direct parallel to quantum optics. The forces are strong, deflecting electrons in much less than a nanometer in some regimes.

ACKNOWLEDGMENTS

We thank Prof. Bert Halperin for many stimulating and informative discussions surrounding the issues raised in this paper. Vaibhav Mohanty helped inspire this work with his work on reference [53]. Discussions with Prof. John H. Miller Jr. were very helpful. We are very grateful to Prof. Peter Milonni for calling our attention to connections between our work and the Hanbury-Brown Twiss literature and its aftermath. We thank the National Science Foundation for supporting this research, through the NSF the Center for Integrated Quantum Materials (CIQM) Grant No. DMR-1231319. AA acknowledges support from Scientific and Technological Research Council of Turkey (TÜBİTAK). JK-R thanks the Emil Aaltonen Foundation for financial support.
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APPENDIX A: More on the Deformation potential

1. General derivation: lattices with non-cubic (or non-square) symmetry

In section IV, we regarded the lattice as having a cubic (or square in 2D) symmetry. However, this is not a serious restriction and can be generalized by starting with more general form of the expansion in Eq. (9):

\[ E(\mathbf{k}; \epsilon_{ij}(\mathbf{r})) = E_0(\mathbf{k}) + \sum_{i,j} E^{ij}_d(\mathbf{k}) \epsilon_{ij}(\mathbf{r}) + \ldots \quad (A1) \]

where \( \mathbf{k} \) is an electron wavevector, \( E_0(\mathbf{k}) \) is band energy of undistorted (hence periodic) lattice, and \( E^{ij}_d(\mathbf{k}) \) are the expansion coefficients of the first order terms. Here, the first-order correction terms in the strain fields, \( \sum_{i,j} E^{ij}_d(\mathbf{k}) \epsilon_{ij}(\mathbf{r}) \), can be considered as the deformation energy. The expansion coefficients \( E^{ij}_d(\mathbf{k}) \) have \( \mathbf{k} \)-dependence, but they can be treated as constants to a good approximation, particularly for non-polar semiconductors [2], and then \( E^{ij}_d \) are called deformation potential constants. Thus, the deformation energy without the \( \mathbf{k} \)-dependence

\[ V_D(\mathbf{r}) = \sum_{i,j} E^{ij}_d \epsilon_{ij}(\mathbf{r}) \quad (A2) \]

is defined as the deformation potential. Eq. (A2) is the generalization of Eq. (10) in the section IV, it does not assume cubic (or square) symmetry. We can reduce Eq. (A2) back to Eq. (10) by considering a lattice with cubic (or square) symmetry where \( E^{ij}_d = 0 \) for \( i \neq j \) and \( E^{ii}_d = E_d \):

\[ V_D(\mathbf{r}) = E_d \nabla \cdot \mathbf{u}(\mathbf{r}) \quad (A3) \]

where \( \sum_i \epsilon_{ii}(\mathbf{r}) = \nabla \cdot \mathbf{u}(\mathbf{r}) \) is dilation.

2. Classical derivation

From the equation (A.28) of Bardeen and Shockley [2], with a bit of generalization, the classical displacement field from a normal mode with a wavevector \( \mathbf{q} \) and a polarization index \( \lambda \) can be written as

\[ \mathbf{u}_{q\lambda}(\mathbf{x}, t) = \epsilon_{q\lambda}(A_{q\lambda} e^{i q \cdot \mathbf{x} - \omega_{q\lambda} t} + A_{q\lambda}^* e^{-i q \cdot \mathbf{x} + \omega_{q\lambda} t}) \quad (A4) \]

where \( \epsilon_{q\lambda} \), \( \omega_{q\lambda} \) and \( A_{q\lambda} \) are polarization unit vector, angular frequency and complex amplitude, respectively, of a normal mode indexed by \( q\lambda \). Note \( \mathbf{x} \) is a spatial coordinate that has nothing to do with electron coordinate \( \mathbf{r} \) so far. The total displacement field is the superposition of the displacement fields from the normal modes.

\[ \mathbf{u}(\mathbf{x}, t) = \sum_{q\lambda} \mathbf{u}_{q\lambda}(\mathbf{x}, t) \]

The Hamiltonian for a normal mode \( q\lambda \) is given by

\[ H_{q\lambda}(t) = \int d\mathbf{x} \left[ \frac{1}{2} \rho \left( \frac{\partial \mathbf{u}_{q\lambda}}{\partial t} \right)^2 + \frac{1}{2} \rho \omega_{q\lambda}^2 |\mathbf{u}_{q\lambda}|^2 \right] \quad (A5) \]

\[ = 2 \rho \omega_{q\lambda}^2 |\mathbf{u}_{q\lambda}|^2 \]

\[ = 2 \rho \omega_{q\lambda}^2 \mathbf{u}_{q\lambda}^2 |A_{q\lambda}|^2 \]
where $\rho_m$ and $V$ are mass density and volume of the solid, respectively. For a system in thermal equilibrium, the average Hamiltonian for each normal mode is given by

$$\langle H_{q\lambda} \rangle_{\text{eq}} = N_{q\lambda} \hbar \omega_{q\lambda}$$

where $N_{q\lambda} = 1/(e^{\hbar \omega_{q\lambda}/k_BT} - 1)$ is Bose occupation. Taking the thermal average value, we obtain

$$|A_{q\lambda}| = \sqrt{\frac{N_{q\lambda}}{2\rho_m V \omega_{q\lambda}}}$$

Also, the phase $\varphi_{q\lambda} = \text{arg}(A_{q\lambda})$ of a normal mode $q\lambda$ can be defined such that $A_{q\lambda} = |A_{q\lambda}| e^{i\varphi_{q\lambda}}$.

In the deformation potential model, the effective potential for the electron at a position $r$ is determined by the strain field exactly at the same position $r$ due to the local approximation. Thus, the classical deformation potential field can be written as

$$V_D(r, t) = E_d \nabla \cdot \mathbf{u}(r, t)$$

where $E_d$ is the deformation potential constant and $l$ stands for longitudinal acoustic mode. Note only longitudinal acoustic modes ($\mathbf{q} \cdot \mathbf{e}_{q\ell} = q$) have a contribution to the deformation potential, not transverse modes ($\mathbf{q} \cdot \mathbf{e}_{q\ell} = 0$), as the transverse modes do not change the interatomic spacing up to the first order in lattice distortion. We use the Debye model that introduces linear dispersion $\omega_{q\ell} = v_s |q|$ where $v_s$ is sound speed and Debye wavenumber (isotropic cutoff) $q_D$. Thus, we obtain the classical deformation potential field

$$V_D(r, t) = -E_d \sum_{q < q_D} \sqrt{\frac{2N_{q\lambda}}{\rho_m V \omega_{q\lambda}}} \sin(\mathbf{q} \cdot \mathbf{r} - \omega_{q\lambda} t + \varphi_{q\lambda})$$

where $\omega_{q\lambda} = v_s q$. Trivially, the phases $\varphi_{q\ell}$ can be redefined to get another equivalent form of the formula, e.g., the one with cosine instead of sine.

### 3. Spatio-temporal autocorrelation function

The spatio-temporal autocorrelation function of the deformation potential gives the strength of the potential fluctuation and the decay of its spatio-temporal correlation:

$$C(\delta r, \delta t) = \langle V_D(r, t)V_D(r + \delta r, t + \delta t) \rangle$$

$$= \langle V_T \rangle^{-1} \int_V \int_0^T dt \langle V_D(r, t)V_D(r, t + \delta t) \rangle$$

$$= \sum_{q \in [q]<q_D} g_q^2 N_q \cos(q \cdot \delta r - \omega_q \delta t)/2$$

$$= \int_{[q]<q_D} \frac{\nu_q}{(2\pi)^d} g_q^2 N_q \cos(q \cdot \delta r - \omega_q \delta t)/2$$

(A6)

where $d$ is the dimension of the considered system. The autocorrelation is significant for spatio-temporal relation $\delta r = v_s \delta t$ corresponding to the sound wave propagation. From the autocorrelation, we can obtain the typical energy scale of the potential fluctuation, i.e., the root mean square of the potential values

$$V_{\text{rms}} = \sqrt{\langle (V_D(r, t))^2 \rangle} = \sqrt{C(0, 0)}.$$  

Note although the electron-phonon coupling amplitude $g_q \sim 1/\sqrt{V}$ has a volume dependence, the potential fluctuation $V_{\text{rms}}$ does not. This is because the number of modes $\sim \sqrt{\nu}$ cancel the volume dependence out as shown in $\nu g_q^2$ factor in Eq. (A6).

For two dimension $d = 2$,

$$C^{(2D)}(\delta r, \delta t) = \int_0^{2\pi} \int_0^\pi \frac{dq_1 dq_2}{(2\pi)^2} \int_0^{3\pi} \frac{d\theta}{\rho_m v_s} \frac{\pi J_0(q\delta r)}{e^{\nu q/\hbar k_BT} - 1} \cos(q_\perp \delta t)$$

where we used

$$\int_0^{\pi} d\theta \cos(A \cos \theta) = \pi J_0(|A|)$$

Spatial autocorrelation function $C^{(2D)}(\delta r, 0)$ is shown in Fig. [4]. Temporal autocorrelation function $C^{(2D)}(0, \delta t)$ is shown in Fig. [12].

For three dimension $d = 3$,

$$C^{(3D)}(\delta r, \delta t) = \int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} \int_0^\pi \frac{d^2 q_1 dq_2}{(2\pi)^3} \int_0^{2\pi} \frac{d\theta}{\rho_m v_s} \frac{2\pi \sin(q_\perp \delta t)}{e^{\nu q/\hbar k_BT} - 1} \cos(v_s q_\perp \delta t)$$

where $\sin(x) = \sin x/x$ for $x \neq 0, \sin(0) = 1$.

### 4. Observation of localized eigenstates

To obtain an eigenstate $\phi_T(E)$ of energy $E$ within the time window $T$, one should calculate the time Fourier transform of the wavefunction [17].

$$|\phi_T(E)\rangle = \frac{1}{\pi \hbar} \int_0^T dt e^{iE t/\hbar} |\psi(t)\rangle$$

(A7)

Also, the time Fourier transform of the autocorrelation function gives spectrum.

$$S_T(E) = \frac{1}{\pi \hbar} \int_0^T dt e^{iE t/\hbar} \langle \psi(0) | \psi(t) \rangle$$

(A8)
where $S_T(E)$ is normalized such that $\int_{-\infty}^{\infty} dE S_T(E) = 1$. Figure 13 shows a localized eigenstate of energy $E = 0.545 V_{\text{rms}}$.

APPENDIX B: Comparison of perturbation theories in coherent state and Fock state pictures

1. Perturbation theory in coherent state picture: elastic scattering

Consider a particle in a potential $V(r)$. The inverse of the transport lifetime (or momentum relaxation time) for an initial state $|k\rangle$ is determined by the sum of the transition rates $\Gamma_{k\rightarrow k'}$ from initial state $|k\rangle$ to any final state $|k'\rangle$ and weighted by the factor $(1 - \cos \theta_{k',k})$ which quantifies how much the momentum autocorrelation decreases for the scattering angle $\theta_{k',k}$ [80].

$$\frac{1}{\tau_{el}} = \sum_{k'} \Gamma_{k\rightarrow k'} (1 - \cos \theta_{k',k})$$

(B1)

where the transition rates are given by Fermi’s golden rule

$$\Gamma_{k\rightarrow k'} = \frac{2\pi}{\hbar} |\langle k'|V|k\rangle|^2 \delta(\varepsilon(k') - \varepsilon(k))$$

and the subscript $\text{el}$ stands for “elastic scattering” ($\varepsilon(k') = \varepsilon(k)$) since in this picture the scattering does not involve any phonon creation or annihilation. Eq. (B1) can be written in terms of the scattering wavevector $q = k' - k$ and the Fourier transform of the potential

$$(k+q|V|k) = \frac{1}{V} \int d\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} V(\mathbf{r}) = \hat{V}(q)$$

Then, Eq. (B1) becomes

$$\frac{1}{\tau_{el}} = \sum_q \Gamma_{k\rightarrow k+q} (1 - \cos \theta_{k,k+q})$$

(B2)

where

$$\Gamma_{k\rightarrow k+q} = \frac{2\pi}{\hbar} |\hat{V}(q)|^2 \delta(\varepsilon(k + q) - \varepsilon(k))$$

We first derive the general formulations in two and three-dimensions for a potential $V(\mathbf{r})$, and the more specific expression for the deformation potential $V_D(\mathbf{r})$ will be established later. Furthermore, we use effective mass model $\varepsilon(k) = \hbar^2 k^2 / 2m^*_e$.

a. 2D

In 2D, Eq. (B2) becomes

$$\frac{1}{\tau_{el}^{(2D)}} = \frac{m^*_e V}{2\pi \hbar^3 k^2} \int_0^{2k} \frac{dq q^2}{\sqrt{1 - (q/2k)^2}} |\hat{V}(q)|^2$$

(B3)

This equation shows only for $q < 2k$, Fourier components of the potential contributes to the transport scattering rate (inverse transport lifetime), and $q > 2k$ Fourier components do not if any. Thus, the wave $|k\rangle$ is “transparent” to the shorter wavelength $q > 2k$, Fourier components of the potential.
As for the deformation potential that we derived before
\[ V_D(r, t; \{ \varphi_p \}) = \sum_{|p| < q_D} 2g_p \sqrt{N_p} \cos (p \cdot r - \omega_p t + \varphi_p) \]
the Fourier transform is
\[ \hat{V}_D(q) = \sum_{|p| < q_D} 2g_p \sqrt{N_p} \int \delta_{p-q,0} e^{i(-\omega_p t + \varphi_p)} + \delta_{p+q,0} e^{-i(-\omega_p t + \varphi_p)} \]
The absolute square of this quantity is
\[ |\hat{V}_D(q)|^2 = 2g^2 q_l \Theta(q_D - q) \] (B4)
where \( \Theta \) is a unit step function. Eq. (B4) shows the deformation potential has nonzero Fourier components for \( q < q_D \). Thus, substituting (B4) into (B3), we obtain the transport scattering rate for the deformation potential in 2D
\[ \frac{1}{\tau_{el}^{(2D)}} = \frac{m^*}{2\pi \hbar^2 k^3} \int_0^{q_{max}} dq q^2 \left( \frac{E^2_q \hbar^2}{\rho_m v_s} e^{\hbar \omega_q / k_{B} T} - 1 \right) \] (B5)
where \( q_{max} = \min\{q_D, 2k \} \).

b. 3D

In 3D, Eq. (B2) becomes
\[ \frac{1}{\tau_{el}^{(3D)}} = \frac{m^* V}{4\pi \hbar^2 k^3} \int_0^{2k} dq q^3 |\hat{V}(q)|^2 \] (B6)

For deformation potential, the Fourier transform was already calculated in (B4) which is valid for any dimension. Thus, substituting (B4) into (B6), we obtain the transport scattering rate for the deformation potential in 3D
\[ \frac{1}{\tau_{el}^{(3D)}} = \frac{m^*}{4\pi \hbar^2 k^3} \int_0^{q_{max}} dq q^3 \left( \frac{E^2_q \hbar^2}{\rho_m v_s} e^{\hbar \omega_q / k_{B} T} - 1 \right) \] (B7)
where \( q_{max} = \min\{q_D, 2k \} \).

c. Considering Fermi statistics

For elastic scattering, the statistical average of a quantity \( Q(\varepsilon) \) depending on electronic energy \( \varepsilon \) considering Fermi statistics is
\[ \langle Q \rangle = \int_0^\infty d\varepsilon \left( -\frac{df}{d\varepsilon} \right) Q(\varepsilon) \]
\[ = \int_0^\infty d(\beta \varepsilon) f(\varepsilon)(1 - f(\varepsilon))Q(\varepsilon) \]
where \( f(\varepsilon) = \frac{1}{e^\lambda - 1 + e^\lambda} \) is Fermi occupation number at electronic energy \( \varepsilon \) and temperature \( T \). The weighting factor is basically the product of the probability \( f(\varepsilon) \) that the initial state of energy \( \varepsilon \) is occupied and the probability \( 1 - f(\varepsilon) \) that the final state of energy \( \varepsilon \) (same as the initial energy because it’s elastic scattering) is unoccupied. Note \( f(\varepsilon)(1 - f(\varepsilon)) \) is narrowly peaked around \( \varepsilon = \mu(T) \) with a characteristic width \( k_B T \), for the temperature \( k_B T \ll E_F \). Note also \( \mu(T) \approx E_F \) for \( k_B T \ll E_F \). Thus, the remaining integrand \( Q(\varepsilon) \) can be expanded at \( \varepsilon = E_F \) and taking the lowest order (zeroth-order) term gives
\[ \langle Q \rangle \approx Q(E_F) \int_0^\infty d(\beta \varepsilon) f(\varepsilon)(1 - f(\varepsilon)) = Q(E_F) \]
for \( k_B T \ll E_F \), i.e., the average only takes the value at the Fermi energy \( E_F \) for \( k_B T \ll E_F \). Thus, \( \frac{1}{\tau_{el}} = \frac{1}{\tau_{el}^{(2D)}} \) for \( k_B T \ll E_F \), i.e., considering Fermi statistics leads to evaluating the transport scattering rate only at Fermi energy \( E_F \) for \( k_B T \ll E_F \) for elastic scattering. Thus, putting \( k = k_p \) into the Eq. (B5) and (B7) is enough for considering Fermi statistics.

2. Perturbation theory in Fock state picture:

inelastic scattering

Consider a scattering of an initial many-body eigenstate \( |k,n\rangle \), labeled by the electron wavevector \( k \) and a collection of phonon occupation numbers \( n = (\ldots, n_q, \ldots) \) from normal modes \( q \lambda \)'s, by the quantum deformation field \( V_D \) defined in Eq. (12). The inverse of the transport lifetime (or momentum relaxation time) for the initial state \( |k,n\rangle \) is determined by the sum of the transition rates \( \Gamma_{k,n \rightarrow k',n'} \) from initial state \( |k,n\rangle \) to any final state \( |k',n'\rangle \) and weighted by the factor \((1 - \cos \theta_{k',k})\).
\[ \frac{1}{\tau_{in}} = \sum_{k',n'} \Gamma_{k,n \rightarrow k',n'} (1 - \cos \theta_{k',k}) \] (B8)
where the transition rates are given by Fermi’s golden rule
\[ \Gamma_{k,n \rightarrow k',n'} = \frac{2\pi}{\hbar} |\langle k',n' | \hat{V}_D | k,n \rangle|^2 \delta(\varepsilon(k',n') - \varepsilon(k,n)) \]
and the subscript \( in \) stands for “inelastic scattering” which will be described below and
\[ \varepsilon(k,n) = \frac{\hbar k^2}{2m^*} + \sum_{q \lambda} \hbar \omega_q \lambda (n_q \lambda + 1/2) \]
is many-body eigenvalue for \( |k,n\rangle \). Then, the Eq. (B8) can be written in terms of the scattering wavevector \( q \).
\[ \frac{1}{\tau_{in}} = \sum_q \left[ \Gamma^{(1)}_{k \rightarrow k+q} (1 - \cos \theta_{k,k+q}) + \Gamma^{(2)}_{k \rightarrow k-q} (1 - \cos \theta_{k,k-q}) \right] \] (B9)
where

\[ \Gamma^{(1)}_{k-k+q} = \frac{2\pi}{\hbar} |g_q|^2 n_q \delta(\varepsilon(k + q) - \varepsilon(k) - \hbar \omega_{ql}) \]

\[ \Gamma^{(2)}_{k-k-q} = \frac{2\pi}{\hbar} |g_q|^2 (n_q + 1) \delta(\varepsilon(k - q) - \varepsilon(k) + \hbar \omega_{ql}) \]

are scattering rates associated with phonon annihilation and creation, respectively, and \( g_q = q \Theta(qD - q) \) is electron-phonon coupling strength including the Debye cutoff \( qD \). Note inelastic scattering \((\varepsilon(k \pm q) = \varepsilon(k) \pm \hbar \omega_{ql})\) naturally came out due to the creation and annihilation operators in Eq. (12). This is in contrast to the perturbation theory in coherent state picture in Eq. (B2) where elastic scattering naturally came out. Also, we will use the thermal average value for \( n_{q\lambda} \):

\[ \langle n_{q\lambda} \rangle_{th} = N_{q\lambda}. \]

In quasielastic approximation, phonon energies are far smaller than the electronic energies so that the electronic energy remains almost the same after creating or annihilating a phonon \( \hbar \omega_{ql} \ll \varepsilon(k') - \varepsilon(k) \). In this approximation, the inelastic scattering matrix element \(|g_q|^2 \delta(\varepsilon(k \pm q) - \varepsilon(k) \mp \hbar \omega_{ql})\) does not differ much from the elastic scattering matrix element \(|g_q|^2 \delta(\varepsilon(k \pm q) - \varepsilon(k))\). Thus, Eq. (B9) becomes

\[ \frac{1}{\tau_{in}} \approx \frac{2\pi}{\hbar} \sum_{q} |g_q|^2 (2N_{q\lambda} + 1) \delta(\varepsilon(k + q) - \varepsilon(k)) \times (1 - \cos \theta_{k,k+q}) \] (B10)

Compare this result the elastic scattering result in Eq. (B2) and (B4)

\[ \frac{1}{\tau_{el}} \approx \frac{2\pi}{\hbar} \sum_{q} |g_q|^2 2N_{q\lambda} \delta(\varepsilon(k + q) - \varepsilon(k)) \times (1 - \cos \theta_{k,k+q}) \] (B11)

The difference between Eq. (B10) and (B11) is only in the addend 1 (related to spontaneous emission of phonon by vacuum) in the integrand, meaning that both the coherent and Fock state pictures (with quasielastic approximation) give consistent results.

### a. Considering Fermi statistics

For inelastic scattering, the average considering Fermi statistics is

\[ \left\langle \frac{1}{\tau_{in}} \right\rangle = \beta \int_{0}^{\infty} d\varepsilon(k) \sum_{k'} \Gamma^{(1)}_{k-k+q} (1 - \cos \theta_{k,k+q}) f(\varepsilon(k)) (1 - f(\varepsilon(k) + \hbar \omega_{ql})) 
+ \Gamma^{(2)}_{k-k-q} (1 - \cos \theta_{k,k+q}) f(\varepsilon(k)) (1 - f(\varepsilon(k) - \hbar \omega_{ql})) \] (B12)

In the quasielastic approximation, \( f(\varepsilon(k))(1 - f(\varepsilon(k) \pm \hbar \omega_{ql})) \) is narrowly peaked around \( \varepsilon(k) \approx \mu(T) \) with a characteristic width \( k_B T \), for the temperature \( k_B T < E_F \). Note also \( \mu(T) \approx E_F \) for \( k_B T \ll E_F \). Thus, the remaining integrand can be expanded at \( \varepsilon(k) = E_F \) (or \( k = k_F \)) and taking the lowest order (zeroth-order) term gives

\[ \left\langle \frac{1}{\tau_{in}} \right\rangle = \sum_{q} \Gamma^{(1)}_{k-k+q} |\varepsilon(k) = E_F| (1 - \cos \theta_{k,k+q}) g(\hbar \omega_{ql}) + \Gamma^{(2)}_{k-k-q} |\varepsilon(k) = E_F| (1 - \cos \theta_{k,k+q}) g(-\hbar \omega_{ql}) \] (B13)

where

\[ g(u) = \int_{0}^{\infty} d(\beta \varepsilon) f(\varepsilon)(1 - f(\varepsilon + u)) \]

\[ \approx \int_{-\infty}^{\infty} d(\beta \varepsilon) f(\varepsilon)(1 - f(\varepsilon + u)) = \frac{e^{\beta u} \beta u}{e^{\beta u} - 1} \]

Considering Fermi statistics gave additional \( g(\pm \hbar \omega_{ql}) \) factor in Eq. (B13) compared to Eq. (B9). Using \( g(\hbar \omega_{ql}) = (N_{q\lambda} + 1)\beta \hbar \omega_{ql} \) and \( g(-\hbar \omega_{ql}) = N_{q\lambda} \beta \hbar \omega_{ql} \),
and quasielastic approximation, from Eq. \[[B13]\] we obtain
\[
\frac{1}{\tau_{\text{in}}} \approx \frac{2\pi}{\hbar q} \sum_{q} \left| g_{q} \right|^{2} 2N_{q}(N_{q} + 1)\beta \omega_{q}(1 - \cos \theta_{k,k+q}) \\
\times \delta(\varepsilon(k + q) - \varepsilon(k))|e(k) = E_{F}
\]
(B14)

Thus, inelastic scattering result in Eq. \[[B14]\] has additional \((N_{q} + 1)\beta \omega_{q}\) factor compared to the elastic scattering result in Eq. \[[B11]\] evaluated at \(\varepsilon(k) = E_{F}\) (or \(k = k_{F}\)).

In 2D, from Eq. \[[B14]\] we obtain
\[
\frac{1}{\tau_{\text{in}}^{(2D)}} \approx \frac{m^{*}}{4\pi \hbar k_{F}^{2}} \int_{0}^{q_{\text{max}}} \frac{dqq^{2}E_{q}^{2}\hbar q}{\sqrt{1 - (q/2k_{F})^{2}}} \rho_{m}v_{s} \\
\times N_{q}(N_{q} + 1)\beta \omega_{q}
\]
(B15)

which is basically the formula derived and used by Hwang and Das Sarma \[[118]\], and Efetov and Kim \[[119,120]\].

To explicitly connect this to the resistivity result, use the relation \(\Delta \rho^{(2D)}(T) = \frac{m^{*}}{e^{2}} \frac{1}{\tau_{\text{in}}^{(2D)}}\) where \(k_{F}^{2} = \pi n\), \(q_{\text{max}} = 2k_{F}\) and \(m^{*}v_{F} = \hbar k_{F}\) for graphene (they also considered absence of backscattering due to chiral nature of the carriers in graphene, which leads to additional factor of \(1 - (q/2k_{F})^{2}\) in the integrand in Eq. \[[B15]\]).

In 3D, from Eq. \[[B14]\] we obtain
\[
\frac{1}{\tau_{\text{in}}^{(3D)}} = \frac{m^{*}}{4\pi \hbar k_{F}^{3}} \int_{0}^{q_{\text{max}}} dqq^{2}E_{q}^{2}\hbar qN_{q}(N_{q} + 1)\beta \omega_{q}
\]
(B16)

which is basically the Bloch-Grüneisen formula \[[7]\]. To explicitly connect this to the resistivity result in the citation, use the relation \(\Delta \rho^{(3D)}(T) = \frac{m^{*}}{e^{2}} \frac{1}{\tau_{\text{in}}^{(3D)}}\) where
\[n = \frac{k_{F}^{2}}{8\pi^{2}}, \quad q_{\text{max}} = q_{D}\] and \(m^{*}v_{F} = \hbar k_{F}\) for normal metals.

3. Comparison of the two pictures

It can be explicitly seen that the inelastic scattering results in Eq. \[[B15]\] and \[[B16]\] have additional \((N_{q} + 1)\beta \omega_{q}\) factor compared to the elastic scattering result in Eq. \[[B5]\] and \[[B7]\] evaluated at \(\varepsilon(k) = E_{F}\) (or \(k = k_{F}\)), which is the difference between the coherent state and Fock state pictures. This factor is unitless and larger than 1, i.e., \((N_{q} + 1)\beta \omega_{q} > 1\) for \(\beta \omega_{q} > 0\).

In the high temperature limit where all the phonon energies are small compared to thermal energy, the factor becomes \(\lim_{T \to 0}(N_{q} + 1)\beta \omega_{q} = 1\), so there is no difference between the two pictures in high temperature limit within the perturbation theory.

There is a distinguishable difference in the low temperature part; both give the correct temperature dependence, but their proportionality constants differ. The inelastic inverse momentum relaxation time is four (five) times larger than that of elastic in 2D (3D). Four (five) times could be a significant difference, but in terms of fitting the experimental data, it is not clear which curve is better. As long as both give the correct temperature dependence in low and high temperature limits, the parameter (in this case the deformation potential constant) can be chosen to fit the experimental data better.

In summary, although the difference in the integrands exists, they both give correct temperature dependence \((1/\tau) \sim T^{4} (T^{5})\) for \(T \ll T_{c}\) in 2D (3D), \(1/\tau \sim T\) for \(T \gg T_{c}\) where \(T_{c} = \min\{T_{BG}, T_{D}\}\).

APPENDIX C: Semiclassical dynamics on the deformation potential: Ray trajectories

1. Semiclassical dynamics on the deformation potential

In the classic solid state textbook by Ashcroft and Mermin \[[3]\], two chapters are devoted to “semiclassical” methods, by which is meant treating external fields acting on electrons in metals as classical fields, with the kinetic part of the Hamiltonian governed by the band structure. Consider a metal at zero Kelvin. For a given electronic band structure \(E_{0}(k)\), the electron group velocity is \(d\mathbf{v}/dt = \partial E_{0}(k)/\partial |\mathbf{k}|\); \(\mathbf{r}\) and \(\mathbf{h}\) are single electron position and momentum, respectively. If there are externally applied electric and magnetic fields \(\mathbf{E}\) and \(\mathbf{B}\), the traditional phenomenological semiclassical model gives \(d(\mathbf{h})/dt = -e[\mathbf{E}(\mathbf{r}, t) + \mathbf{r} \times \mathbf{B}(\mathbf{r}, t)]\) \[[5,121]\]. Consequently, electron motion is treated classically. This is an \textit{ad hoc} idea, but it works extremely well.

A crucial observation is that, for \(2k_{F} \gg q(T)\), electrons are in a semiclassical regime with respect to the deformation potential, having short Fermi wavelengths compared to the length scale of the deformation potential. This supports the idea that the deformation potential \(V_{D}(\mathbf{r}, t)\) can be considered as a classical field acting on the electrons, just as external fields are treated. Then, Hamiltonian is given as \(H(\mathbf{h}, \mathbf{r}, t) = E_{0}(\mathbf{k}) + V_{D}(\mathbf{r}, t)\).

We expect the (phenomenological) Hamilton’s equations of motion to be
\[
\frac{d(\mathbf{h})}{dt} = -\frac{\partial H(\mathbf{h}, \mathbf{r}, t)}{\partial \mathbf{r}}; \quad \frac{d\mathbf{r}}{dt} = \frac{\partial H(\mathbf{h}, \mathbf{r}, t)}{\partial (\mathbf{h})}.
\]
(C1)

This allows use of nonperturbative semiclassical trajectory based methods, just as external electromagnetic fields are routinely treated \[[5,121]\].

We numerically investigate the electron scattering by the deformation potential using a fourth-order symplectic scheme for integration \[[122]\]. For each temperature, we run thousands of trajectories with the same initial kinetic energy \(E_{F}\), using random initial directions and positions, and several realizations of the random deformation potential. Then, average momentum relaxation time can be calculated from the simulation results.
V parameters, the fluctuation of the deformation potential can be calculated analytically using classical perturbation theory. One knows $\delta \mathbf{p}(t) = \mathbf{p}(t) - \mathbf{p}(0) = \int_0^t dt' \left( -\frac{\partial V_D(r(t'))}{\partial r(t')} \right)$. Then, $\mathbf{p}(0) \cdot \mathbf{p}(t) = |\mathbf{p}(0)||\mathbf{p}(t)| \cos \chi(t) \approx |\mathbf{p}(0)|^2 \left( 1 - \frac{\langle |\delta \mathbf{p}(t)|^2 \rangle}{2|\mathbf{p}(0)|^2} \right)$ where $\chi(t)$ is the angle between the two momenta, and the quasielasticity of scattering $|\mathbf{p}(t)| \approx |\mathbf{p}(0)|$.

Take the ensemble average (average over all possible realizations of deformation potentials specified by $\{\varphi_q\}$) to obtain $\langle c(t) \rangle = \langle \mathbf{p}(0) \cdot \mathbf{p}(t) \rangle = |\mathbf{p}(0)|^2 \left( 1 - \frac{\langle |\delta \mathbf{p}(t)|^2 \rangle}{2|\mathbf{p}(0)|^2} \right)$ where $\langle |\delta \mathbf{p}(t)|^2 \rangle = E_d^2 \sum_q \frac{2\hbar q}{\rho_m v_F} \left( \frac{q \mathbf{p}(0)}{m^*} \right)^2 \frac{1 - \cos q(\mathbf{p}(0)/m^*)}{e^{hqv_F/k_BT} - 1}$ using unperturbed trajectory $\mathbf{r}^{(0)}(t') = \mathbf{r}(0)t'/m^*$. Note that the sinusoidal oscillation with different phases vanishes due to the ensemble average, i.e., $\langle \cos(A + \varphi_q) \cos(B + \varphi_q) \rangle = \delta_{AB} \langle \cos(A + \varphi_q) \cos(B + \varphi_q) \rangle$.

In the 2D case, we can use polar coordinates for $\mathbf{q}$ where angle $\theta$ is chosen such that $\mathbf{q} \cdot \mathbf{p}(0) = q|\mathbf{p}(0)| \sin \theta$, and use $|\mathbf{p}(0)| = m^*v_F$, then

$$\langle |\delta \mathbf{p}(t)|^2 \rangle = E_d^2 \int_0^{\pi} dq q \frac{2\hbar q}{\rho_m v_F} \left( \frac{1}{v_F \sin \theta} \right)^2 \times \frac{1 - \cos(qv_F t \sin \theta)}{e^{hqv_F/k_BT} - 1}$$

where $f(A) = A\pi \{J_1(A)[-2 + A\pi H_0(A)] + A J_0(A)[2 - \pi H_1(A)]\}$ and $H$'s and $J$'s are Struve and Bessel functions, respectively. Looking at sufficiently long time correlation such that $A = qv_F t \gg 1$ holds, we can approximate $f(A) \approx 2\pi A$. Then, we obtain momentum relaxation time $\tau$ from $\langle c(t) \rangle = |\mathbf{p}(0)|^2 (1 - t/\tau)$ for $t \ll \tau$, and obtain inverse momentum relaxation time

$$\frac{1}{\tau_{cl}^{(2D)}} = \frac{m^*}{2\pi \hbar^3 k_F^3} \int_0^{\pi} dq q^2 E_d^2 hq \frac{1}{\rho_m v_F e^{hqv_F/k_BT} - 1} \tag{C2}$$

where the subscript $cl$ stands for “classical,” and used $|\mathbf{p}(0)| = m^*v_F = \hbar k_F$. Eq. (C2) does not have a geometrical factor $\sqrt{1 - (q/2k_F)^2}$ appearing in the quantum elastic perturbation theory in Eq. (B5), but other than that the other parts of the integrand is the same. This shows classical-quantum correspondence. Likewise, in 3D, we obtain

$$\frac{1}{\tau_{cl}^{(3D)}} = \frac{m^*}{4\pi \hbar^3 k_F^3} \int_0^{\pi} dq q^3 E_d^2 hq \frac{1}{\rho_m v_F e^{hqv_F/k_BT} - 1} \tag{C3}$$

Eq. (C3) has the same integrand as the quantum elastic perturbation theory in Eq. (B7), showing classical-quantum correspondence. However, note that the integration range of classical results in Eq. (C2) and (C3) is

![FIG. 14. Deformation potential and semiclassical ray trajectories at two different temperatures 4K and 8K for graphene [119]. In blue tones, ensembles of classical electron pathways launched uniformly over a small range of angles revealing branched flow. Identical random phases are used to generate the deformation potential for both temperatures. It shows the emergence of new vibrational modes with increasing temperature. The bumps and dips also get higher and deeper with increasing temperature.](image)
upto $q_D$, in contrast to $q_{\text{max}}$ in quantum results in Eq. (B5) and (B7). This means that, unlike in quantum mechanics, there is no “transparency” to $q_{\text{max}} < q < q_D$ components of the potential in classical mechanics. This difference will not be problematic if one uses classical simulation only in semiclassical regime $2k_F \ll q_D$ where $q_{\text{max}} = q_D$. 