Renormalization group method based on the ionization energy theory

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Proofs are developed to explicitly show that the ionization energy theory (IET) is a renormalized theory, which mathematically exactly satisfies the renormalization group formalisms developed by Gell-Mann-Low, Shankar and Zinn-Justin. However, the cutoff parameter for IET relies on the energy-level spacing, instead of lattice spacing in $k$-space. Subsequently, we apply the earlier proofs to prove that the mathematical structure of the ionization-energy dressed electron-electron screened Coulomb potential is exactly the same as the ionization-energy dressed electron-phonon interaction potential. The latter proof is proven by means of the second-order time-independent perturbation theory with the heavier effective mass condition, as required by the electron-electron screened Coulomb potential. The outcome of this proof is that we can derive the heat capacity and the Debye frequency as a function of ionization energy, which can be applied in strongly correlated matter and nanostructures.

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I. INTRODUCTION

The specific application of the renormalization group theory (RGT) in high energy physics requires removing the ultraviolet ($k \to \infty$) divergences, where $k$ is a wavenumber. Whereas, in condensed matter physics, RGT applies to the study of phase transitions of spin-dependent (magnetic) system and removing infrared ($k \to 0$) divergences. For example [1], in a $d$-dimensional integral,

$$
\int_{0}^{\Lambda} \frac{d^dk}{k^2 + m^2} = \int_{0}^{\Lambda} \frac{k^{d-1}dk}{k^2 + m^2} \propto \begin{cases} 
\Lambda^{d-2} & \text{for } d > 2 \\
\ln \Lambda & \text{for } d = 2
\end{cases} \text{ for } d < 2,
$$

(1)

where $\Lambda$ is a cutoff parameter in a reciprocal space ($\pi/a$). For large $\Lambda/m^2$ and $d > 2$, Eq. (1) diverges like $\Lambda^{d-2}$ in the limit, $\Lambda \to \infty$ (ultraviolet divergence). Here, $m$ denotes mass and note that it is common in the high-energy physics literature to take $\hbar = c = 1$, where $\hbar$ and $c$ are the Planck constant divided by $2\pi$ and the speed of light in vacuo, respectively. Therefore, $k^2 + m^2 \equiv c^2 \hbar^2 k^2 + m^4 = E^2$. On the other hand, for $d \leq 2$ and $m = 0$, the integral diverges like $\ln \Lambda$ ($d = 2$) and $\frac{\Lambda^{d-2}}{d-2}$ ($d < 2$) as $\Lambda \to 0$ (infrared divergence). Hence, it is appropriate to start with a general formalism of RGT (given below) based on the work of Zinn-Justin [2] and Goldenfeld [3]. From this general approach, we will be able to identify the relation between IET and RGT, which will be discussed in the subsequent sections.

A. General formulation: Zinn-Justin formalism

The renormalization procedure originated as an empirical program to overcome the problem of infinities (singularities) in quantum electrodynamics [2]. The renormalization procedures have enabled one to calculate finite values from divergent expressions. In addition, the predicted finite values obtained from these renormalized results have been confirmed by experiments with high precision, which eventually gave birth to the formal RGT as it is known today [2]. In the subsequent sections, the RGT is introduced by means of the Hamiltonian flow. This means that the original Hamiltonian is renormalized with an arbitrary cutoff parameter, $\Lambda$, and then, in the final formula, $\Lambda$ is removed via the limits, $\Lambda \to 0$ or $\Lambda \to \infty$. All these will be clarified shortly.

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1. Hamiltonian flow

We first introduce the parameter, $\Lambda$, which is the dilatation parameter in such a way that the effective Hamiltonian is given by $H_\Lambda$. Therefore, $H \mapsto H_\Lambda$ where $H_\Lambda$ is the renormalization group (RG) transformed Hamiltonian \cite{2} and $\mapsto$ denotes mapping or creating (within the Hamiltonian space) a function $H_\Lambda$ from $H$ that depends on $\Lambda$ explicitly. In this case, the RG idea is that the bare Hamiltonian, $H = H_{\Lambda=1} = H_1$, while the RG transformed Hamiltonian ($H_\Lambda$) and for $\Lambda > 0$, we need to know the flow of the $H_\Lambda$. The general form of the flow equation is given by \cite{2}

$$\Lambda \frac{d}{d\Lambda} H_\Lambda = \mathcal{T}[H_\Lambda], \quad (2)$$

where $\mathcal{T}$ is the transformation in the space of the Hamiltonian. We assume \cite{2} that the transformation is Markovian in which, the transformation does not depend on the trajectory between $H$ and $H_\Lambda$. In addition, the Markovian process is stationary, meaning that the right-hand side (RHS) of Eq. (2) is not an explicit function of $\Lambda$, but only through $H_\Lambda$. Moreover, the identity,

$$\Lambda \frac{d}{d\Lambda} = \frac{d}{d \ln \Lambda},$$

will be used without warning from now onwards. Here, Eq. (2) is a RG equation in which $\Lambda$ determines the scale changes in the dynamical process. A fixed point can be defined as independent of $\Lambda$ where we label $H^*$ as the Hamiltonian at a fixed point, in which Eq. (2) can be written as \cite{2}

$$\Lambda \frac{d}{d\Lambda} H^*_\Lambda = \mathcal{T}[H^*_\Lambda] = 0. \quad (3)$$

Let us now work near a fixed point, in other words, we can perform linearization: $H_\Lambda = H^* + \Delta H_\Lambda$. Linearizing Eq. (2) leads us to \cite{2}

$$\Lambda \frac{d}{d\Lambda} \Delta H_\Lambda = \mathcal{L}^*(\Delta H_\Lambda), \quad (4)$$

where $\mathcal{L}^*$ is a linear operator independent of $\Lambda$. The solution to Eq. (1) is \cite{2}

$$\Delta H_\Lambda = \Lambda \mathcal{L}^* \Delta H_{\Lambda=1}, \quad (5)$$

from Eq. (6), it is possible to study the RG flow near the fixed point where Eq. (5) gives us the relationship between the transformed Hamiltonian, $\Delta H_{\Lambda\neq1}$ somewhere in the neighborhood of $H^*$ and $\Delta H_1$, also in the neighborhood of $H^*$. The fixed points are also known as the critical (fixed) points where the fixed-point Hamiltonian ($H^*$) is invariant to $\Lambda$. For example, there are two trivial critical points for a ferromagnet, for $T = 0$ (all spins are aligned) and for $T \to \infty$ (all spins are randomly oriented). The non-trivial critical point is for $T = T_C$ where, below $T_C$, some spins are aligned that gives rise to the correlation length. The correlation length is defined as the length for a group of spins that are aligned below $T_C$. Any RG transformations must give same results at $T = 0$ (ordered) and for $T \to \infty$ (disordered).

**Note 1:** Every solution obtained from the IET Hamiltonian, is a renormalized solution (can be proven using the Zinn-Justin general formalism given above.)

2. Classification of eigenvectors

Assuming \cite{2} that $\mathcal{L}^*$ has discreet spectra with eigenvalues, $l_i$, which corresponds to a set of eigenvectors, $\mathcal{Y}_i$. Therefore, one can expand $\Delta H_\Lambda$ on the eigenvectors, $\mathcal{Y}_i$ of $\mathcal{L}^*$:

$$\Delta H_\Lambda = \sum_i h_i(\Lambda) \mathcal{Y}_i. \quad (6)$$
The flow equation, Eq. (11) is now given by

\[ \Lambda \frac{d}{d\Lambda} h_i(\Lambda) = l_i h_i(\Lambda), \]  

(7)

which has the solution,

\[ h_i(\Lambda) = \Lambda^{l_i} h_i(1), \]  

(8)

Here, the eigenvectors, \( \mathcal{Y}_i \) can be classified according to the sign on the eigenvalues, \( l_i \), provided that \( \Lambda > 0 \), which is true in our case because, \( 1 \leq \Lambda \leq \infty \). Note here that we deliberately chose the lower limit \( \Lambda = 1 \), and not \( \Lambda = 0 \) as mentioned previously. This choice does not affect the physical theory in any way since we can set any arbitrary values for \( \Lambda \), which are convenient to us so as to capture the required physics accurately. Furthermore, in this case, setting \( \Lambda = 0 \) is meaningless as can be seen from Eq. (8). Having explained that, now we can return to the classification issue, which are given by:

(i) \( l_i > 0 \): \( h_i \) and the components of \( h_i \) will grow or increase with \( \Lambda \), and the system moves away from the fixed point Hamiltonian, \( H^* \) (repelling or unstable fixed point). In this case, \( h_i \) is said to be relevant because increasing \( \Lambda \) (increasing dilatation) decreases effective correlation length. For example, the Curie temperature of a ferromagnet is an unstable critical fixed point, which means that any slight deviation from this point will lead the system away, toward the stable fixed points. The stable fixed points here are for \( T > T_C \) (paramagnet: disordered spins) or \( T < T_C \) (ferromagnet: increasing ordering of spins).

(ii) \( l_i < 0 \): \( h_i \) and the components of \( h_i \) decreases with \( \Lambda \). Thus giving rise to irrelevant \( h_i \) because larger \( \Lambda \) also implies larger correlation length. Here, the system moves toward a fixed point (attractive or stable fixed point). The fixed points at \( T = 0(\langle T_C \rangle) \) and \( T = \infty(\langle T_C \rangle) \) stated above are stable fixed points.

(iii) \( l_i = 0 \) (vanishing eigenvalues): \( h_i \) is called a marginal variable. In this case, one needs to expand Eq. (11) beyond the linear approximation (which was carried out earlier). Hence, Eq. (7) can be written as

\[ \Lambda \frac{d}{d\Lambda} h_i(\Lambda) \propto B h_i^2(\Lambda), \]

(9)

where \( \pm B \) (constant) leads to marginally stable \((+B)\) and unstable fixed points \((-B)\). For \( +B \) and \( \Lambda \to \infty \), the solution behaves like

\[ h_i(\Lambda) \propto -\frac{1}{B \ln \Lambda}. \]

(10)

(iv) The eigenvectors that do not affect the physical properties or the components of \( h_i \) are called redundant. In other words, redundant eigenvectors give only multiplicative constants.

B. Coulomb screening: Shankar formalism

We start by first giving a simple but very important example of renormalization, where the Thomas-Fermi screened Coulomb and the bare Coulomb potentials are actually renormalized potentials. We follow the field theory formalism provided by Shankar, but the notations follow Ref. for easy comparison with the IET. In the field theory approach, the Coulomb potential, after introducing a smooth cutoff, \( \exp[|k|/\Lambda] \) is given by

\[ V(k, \Lambda) = \frac{e^2}{\epsilon_0 \left[ k^2 + \frac{k}{\Lambda + K_s^2} \right]}, \]

(11)

where \( K_s \) is the Thomas-Fermi wavenumber and \( k \) is the wavenumber. It is straightforward to note here that \( V(k, 0) \) gives the Thomas-Fermi screened Coulomb potential,

\[ V(k, 0) = \frac{e^2}{\epsilon_0 (k^2 + K_s^2)}, \]

(12)
whereas, $V(k, \infty)$ leads to the bare Coulomb potential,

$$V(k, \infty) = \frac{e^2}{\epsilon_0 k^2},$$  \hspace{1cm} (13)$$

Here, $\Lambda$ is a cutoff parameter that has a dimension of $k$, and it is necessary to eliminate it from the final formula, either by taking $\Lambda \to \infty$ or $\Lambda \to 0$ as carried out above. The reason for doing so is that the final formula cannot be a function of the artificially introduced cutoff parameter, $\Lambda$. In the intermediate regime, $k \ll \Lambda \ll (K^2_s/k)$, Eq. (11) is given by

$$V(k, \Lambda) \approx \frac{e^2 \Lambda}{\epsilon_0 kK^2_s},$$  \hspace{1cm} (14)$$

which describes the direct proportionality between $V(k, \Lambda)$ and $\Lambda$. This relation is very important to understand the formalism of IET with respect to RGT.

**Note 2:** We will show how the IET can be used to capture the relationship between $V(k, \Lambda)$ and $\Lambda$. A direct proof is given that formally associate the IET with the general formulation of RGT, as discussed earlier. The renormalized screened Coulomb potential, $V_{sc}$ plays the pivotal role with respect to strong $e-e$ and $e-ph$ interactions.

### C. Renormalization group equation: Gell-Mann–Low formalism

The Gell-Mann-Low equation is also known as the $\beta$-function, or the differential RG transformation, is the principal result of the RG analysis [3]. In fact, we have already introduced equations in the form of the Gell-Mann-Low equation many times earlier, which is given in Eqs. (2), (3), (4), (7) and (9). Here, we will derive the equation in a straightforward manner. Assuming that we have a periodic lattice, an arbitrary coupling constant is expected to change or flow with respect to any changes to the cutoff parameter ($\Lambda$) that controls the distance between the lattice points (lattice spacing) or the number of lattice points considered (magnification). For example, one can write the coupling constant ($c$) as

$$c' = c \Lambda^{1-g},$$  \hspace{1cm} (15)$$

where $g = 1$ implies non-interacting case that leaves $c$ unchanged. Furthermore, for $g < 1$ and $g > 1$ one have the repulsive (unstable) and attractive (stable) fixed points, respectively. This can be understood from the classification of eigenvalues discussed above: $g < 1$ gives larger $c$ because

$$c' \propto c \Lambda^{1-g<1}. \hspace{1cm} (16)$$

On the other hand, $g > 1$ gives smaller $c$ due to

$$c' \propto c \Lambda^{1-g<0}. \hspace{1cm} (17)$$

Usually, we need to set a cutoff value such that $\Lambda = \Lambda_{\text{min}} = 0$ or 1 or any finite values. Nevertheless, we will discuss this with respect to the IET in the following section. One then can iterate the RG equation, [Eq. (15)] to explore the sequence, $c', c'', \cdots$, and so on. Each iteration implies a change in the distance between the lattice points (spacing) or the number of lattice points as discussed previously. For example, Eq. (15) can be written as

$$c' = c \Lambda^{1-g},$$

$$\ln c' = \ln c \Lambda^{1-g},$$

$$c' = c e^{\ln \Lambda^{1-g}}.$$  \hspace{1cm} (18)$$

Now, the flow of the coupling constant, $c$ with respect to $\Lambda$ is simply the differential equation given by
\[
\int c' \frac{dc}{c} = (1 - g) \int d \ln \Lambda, \tag{19}
\]
\[
\frac{dc}{d \ln \Lambda} = \Lambda \frac{dc}{d \Lambda} = c(1 - g) = \beta(c), \tag{20}
\]

where this equation is known as the Gell-Mann-Low equation, or also called the beta \((\beta)\) function. All the solutions obtained from the IET Hamiltonian through the ionization energy based Fermi-Dirac statistics satisfy equations identical to Eq. \((20)\).

II. CLAIM AND THE PROOF

From the general formulation, and the renormalized Coulomb screening potential derivation given earlier, we know that there is a relationship between the effective Hamiltonian or \(V(k, \Lambda)\) and the length scale \(\Lambda\) \([2\,–\,4]\), though one should remove it by means of the appropriate limits \([\text{for example, see Eqs. } (12)\,\text{and } (13)]\). In any case, one can actually expose a subtle issue here, which is: for a given system, the \(V(k, \Lambda)\) can be \(\Lambda\)-dependent, which makes it possible to evaluate the evolution of the Coulomb potential between two different systems. For example, substitutional doping of element C into AB \((AB_1-xC_x)\) implies that \(V(k, \Lambda)\) should either be (i) dependent on \(\Lambda\) explicitly (provided that the other microscopic variables such as wavefunctions and \(K_s\) are fixed as constants) or (ii) the Coulomb screening is independent of \(\Lambda\). If it is independent of \(\Lambda\), then we need to know some details of the microscopic variables explicitly for each doping \(x\).

In IET, we have opted for the former strategy \([(i) \Lambda\text{-dependent}], which will be proven here. However, in IET formalism, we will not employ the field-theoretic cutoff-parameter approach since \(\Lambda\) is not only artificial but also microscopically not useful because it does not carry any information about the microscopic details of a particular system. For example, we will never know how to change \(\Lambda\) with increasing \(x\), or for different doping elements.

A. Claim

From our earlier work, the many-electron atomic Hamiltonian is given by \([6]\)
\[
\hat{H} = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 - \frac{e^2}{4\pi \varepsilon_0} \sum_{i \neq j} \left( \frac{Z}{r_i} - \frac{1}{2} \frac{1}{|r_i - r_j|} e^{-\sigma(r_i + r_j)} \right), \tag{21}
\]
where \(m\) is the electron’s mass, \(e\) and \(Z\) are the electron’s charge and atomic number, respectively. Moreover, \(|r_1 - r_2| = \sqrt{r_1^2 + r_2^2 - 2r_1r_2 \cos(\theta_2)}\), while the labels, \(i\) and \(j\) identify the electrons and avoid counting them twice. The last term, which describes the screened \(e\)-\(e\) potential makes the Hamiltonian translationally not invariant for solids. However, the Hamiltonian can be made translationally invariant by assuming the dopants to be distributed homogeneously. For non-homogeneous distribution, we will make use of Eq. \((23)\) (Schrödinger equation with redefined eigenvalue) discussed below where we will leave Eq. \((21)\) for atomic system, as it should be. The \(\sigma\) is given by \([6, 7]\)
\[
\sigma = \mu e^{\frac{1}{2} \lambda (-\xi)}. \tag{22}
\]
Here, \(\mu\) is the screening constant of proportionality, while \(\lambda = (12 \pi \varepsilon_0 / e^2) a_B\), where \(\varepsilon_0\) and \(a_B\) denote permittivity of free space and Bohr radius, respectively. In solids however, the many-body Hamiltonian can be written as \([8]\)
\[
\hat{H} \varphi = (E_0 \pm \xi) \varphi. \tag{23}
\]
In this case, we can prove for atomic system, Eq. \((23)\) is equivalent to Eq. \((21)\) \([8]\). Here, \(\xi\) is the energy needed for a particle to overcome the bound state and the potential that surrounds it. \(E_0\) denotes the total energy at temperature, \(T = 0\). We claim that every solution obtained from the IET Hamiltonian \([\text{Eq. } (21)\] is a renormalized solution, which can be recast into RG differential equation, in the form of the Gell-Mann-Low formula. In order to prove this, we first
need to show that the many-electron Hamiltonian given in Eq. (21) satisfies the Zinn-Justin formalism. Secondly, one also needs to prove that the Shankar Coulomb screening formula given in Eq. (14) satisfies Eq. (24). Once we have done these, then it is straightforward to follow the proof of the claim.

\[ \hat{V}_{\text{sc}} = \frac{e}{4\pi\varepsilon_0} e^{-\mu r e^{\frac{1}{2}\lambda(-c)}} = \frac{e}{4\pi\varepsilon_0} e^{-\sigma r}. \]  

(24)

B. Proof

Let us recall Eqs. (6) and (8), which can be rewritten as [using Eq. (23)]

\[ \Delta H_{\Lambda} = \sum_i h_i(\Lambda)\mathcal{Y}_i, \]

\[ h(\Lambda)\mathcal{Y} = \hat{H}\varphi. \]  

(25)

Here, \( \Delta H_{\Lambda} \) is the slightly deviated Hamiltonian, from the fixed point Hamiltonian (\( H^* \)) via linearization procedure given earlier. In addition, \( \mathcal{Y} \) and \( \varphi \) are the eigenvectors, while \( \Lambda \) is known as the cutoff parameter that defines the RG iterations. We are trying to rewrite the general RG Hamiltonian of Zinn-Justin with the many-electron IET Hamiltonian [Eq. (21)]. In this IET Hamiltonian, the screened e-e interaction Coulomb potential is the one that has been renormalized and therefore, Eq. (25) can be written as

\[ h(\Lambda)\mathcal{Y} = \hat{V}_{\text{sc}}\varphi, \]

\[ h(\Lambda) = \Lambda^l h(1) \Rightarrow \hat{V}_{\text{sc}}(\Lambda) = \Lambda^l \hat{V}_{\text{unsc}}, \]  

(26)

where \( l \) is the eigenvalue (\( l < 0 \): because \( \hat{V}_{\text{unsc}} \) must decrease with \( \Lambda^l \)) that has its origin in the discreet linear operator, \( L^* \) as described in Eq. (4). Here, \( \hat{V}_{\text{unsc}} \) is the unscreened (bare) Coulomb potential that gives the strongest e-e interaction. Comparing Eq. (26) with Eq. (24) leads to the relation

\[ \Lambda_{\text{Zinn}}^l = \Lambda_{\text{Justin}}^l = e^{-\mu r e^{-\frac{1}{2}\lambda c}}. \]  

(27)

Now, taking the limit, \( l \to 0 \) gives \( \Lambda^l \to 1 \), which in turn implies \( \xi \to \infty \) that leads Eq. (26) to

\[ \hat{V}_{\text{sc}}(\Lambda) \to \hat{V}_{\text{unsc}}, \]  

(28)

which is correct based on the IET. On the other hand, the limit, \( l \to l_{\text{max}} \) gives \( \Lambda^l \to \Lambda_{\text{min}} \) (because \( l < 0 \)) that implies \( \xi \to 0 \) and therefore we obtain

\[ \hat{V}_{\text{sc}}(\Lambda) \to \Lambda_{\text{min}}^{l_{\text{max}}} \hat{V}_{\text{unsc}} = \hat{V}_{\text{unsc}} e^{-\mu r}, \]  

(29)

where, this result is also in agreement with the IET. However, for \( l \to -\infty \) gives \( \Lambda^l \to 0 \) that requires \( \mu \to \infty \) and thus Eq. (29) is given by

\[ \hat{V}_{\text{sc}}(\Lambda) \to 0, \]  

(30)

in which, this result satisfies both IET and the original result of the Thomas-Fermi screening.

What we have done thus far is that we have proven that the cutoff parameter, \( \Lambda \) from the Zinn-Justin formalism can be directly related to the IET based screened Coulomb potential as given in Eq. (27). In other words, \( \hat{V}_{\text{sc}}(\Lambda) = \hat{V}_{\text{unsc}} \) is obtained for \( l = 0 \) (\( \Lambda^l = 1 \)) that implies strong correlation between electrons. On the other hand, \( \hat{V}_{\text{sc}}(\Lambda) = \hat{V}_{\text{unsc}} e^{-\mu r} \) is obtained for \( l = l_{\text{max}} \) (\( \Lambda^l = \Lambda_{\text{min}} \)) and subsequently, \( \hat{V}_{\text{sc}}(\Lambda) = 0 \) for \( l \to -\infty \) (\( \Lambda^l \to 0 \)). Therefore, the screened Coulomb potential, \( \hat{V}_{\text{sc}} \) is indeed a renormalized potential, without infinities. Infinites do not arise here due to the definition of Eq. (27). Note here that the limit, \( \xi \to \infty \) implies finite value for \( \hat{V}_{\text{unsc}} \), which in turn gives strictly finite
values for both $l_{\text{max}}$ and $\Lambda_{\text{min}}$. For example, $\hat{V}_{\text{unsc}} e^{-\mu r}$ can be related to the Thomas-Fermi screening potential by identifying $l_{\text{max}} = l_{\text{TF}}$ and $\Lambda_{\text{TF}}^{l_{\text{min}}} = \Lambda_{\text{TF}} = e^{-\mu r}$. Hence, from the IET formalism, we can find the evolution of the cutoff parameter, $\Lambda$ for different doping, $x$ and doping elements.

Now one can proceed to obtain the Gell-Mann-Low equation. Using Eqs. (26) and (27), one can write

\[ \ln \tilde{V} = \ln \Lambda_\ell = -\mu re^{-\frac{1}{2} \lambda \xi}, \]  (31)

\[ \frac{d \ln \tilde{V}}{d \xi} = \frac{1}{2} \lambda \mu re^{-\frac{1}{2} \lambda \xi}, \]  (32)

\[ \frac{d \xi}{d \ln \tilde{V}} = \frac{2}{\lambda \mu re^{-\frac{1}{2} \lambda \xi}}; \]  (33)

where $\ln[\hat{V}_{\text{sc}}/\hat{V}_{\text{unsc}}] = \ln \tilde{V}$. Since $\ln \tilde{V} = \ln \Lambda^l$, we can rewrite Eq. (33) as

\[ \lambda \mu r = 2 \lambda \xi = \beta(\xi), \]  (34)

Equation (34) has exactly the same form as Eq. (20).

The next step is to prove the IET version of the screened Coulomb potential, $\hat{V}_{\text{sc}}$ can be transformed into the form of the Shankar Coulomb screening formula [Eq. (14)]. The Fourier transformed $\hat{V}_{\text{sc}}$ [Eq. (24)] is given by [7]

\[ \hat{V}_{\text{sc}}(k) = \frac{e^2}{\epsilon_0(k^2 + K_s^2 e^{-\lambda \xi})}. \]  (35)

Subsequently, one obtains

\[ \hat{V}_{\text{sc}}(k) = \frac{e^2}{\epsilon_0 e^{-\lambda \xi} \left[ \frac{k^2}{e^{-\lambda \xi}} + K_s^2 \right]} \approx \frac{e^2 \Lambda}{\epsilon_0 K_s^2}. \]

or

\[ \hat{V}_{\text{sc}}(k) \approx \frac{e^2 \Lambda}{\epsilon_0 K_s^2}. \]  (36)

where, the limit $k^2 \ll K_s^2 e^{-\lambda \xi}$ has been invoked. Therefore, one obtains the relation,

\[ \Lambda_{\text{IET}} = e^{\lambda \xi}, \]  (37)

from Eq. (36). Comparison between Eq. (36) and Eq. (14) gives

\[ \Lambda_{\text{Shankar}} = k \Lambda_{\text{IET}}. \]  (38)

Hence, Eq. (38) is the relation between the Shankar cutoff parameter and the IET-based cutoff parameter, where $\Lambda_{\text{IET}}$ is a function of the ionization energy or the energy-level difference ($\xi$) of the constituent atoms in strongly correlated matter. Importantly, when $\Lambda \to \infty$, then we have $\hat{V}_{\text{sc}}(k) \to \infty$, which is also in accordance with the limit, $\xi \to \infty$, as it should be. This divergence, $\hat{V}_{\text{sc}}(k) \to \infty$ is entirely due to the inequalities, $k^2 \ll K_s^2 e^{-\lambda \xi}$ (for $\Lambda_{\text{IET}}$) and $k \ll \Lambda_{\text{Shankar}} \ll (K_s^2/k)$. Having found Eq. (38), one can go on to prove that every solution of Eq. (23) is a
renormalized solution. In fact, one just has to repeat the proof given below for every physical variable that has this exponential factor. However, we will only work out the proof for the $\hat{V}_\text{sc}$ here, where this procedure can be easily carried out for other physical variables.

Now one can proceed to obtain the Gell-Mann-Low equation as follows: Eq. (24) can also be written as

$$\hat{V}_\text{sc} = \frac{e^4}{4\pi\varepsilon_0 r} e^{-\mu r} e^{-\frac{1}{2}\lambda \xi} = \hat{V}_\text{unsc} e^{-\mu r}/\Lambda^{1/2},$$

where Eqs. (36) and (39) give us the procedure to recover the exponential function with the same mathematical structure as the Shankar smooth cutoff [4], which is given by $\exp[-|k|/\Lambda]$. Note however, $\Lambda_{\text{IET}}$ is always dimensionless and refers to the distance between energy levels, unlike $\Lambda_{\text{Shankar}}$ that has wavenumber dimension and is based on the distance between the lattice points. Finally, one can derive the Gell-Mann-Low differential equation from Eq. (40) as given below

$$\frac{d\ln \hat{V}}{d\xi} = \frac{1}{2} \lambda \mu r e^{-\frac{1}{2} \lambda \xi},$$

$$\frac{d\xi}{d\ln V} = \hat{V} \frac{d\xi}{dV} = \frac{2}{\lambda \mu r e^{-\frac{1}{2} \lambda \xi}} = \beta(\xi),$$

Equation (42) has exactly the same form as Eq. (34). Now, we can repeat the procedure between Eq. (39) and Eq. (42) to obtain the Gell-Mann-Low differential equation for various physical variables mentioned previously.

Equation (42) also tells us that the flow of $\xi$ is determined by the changes in the physical parameter, $\hat{V}$. From the IET, we know how the changes in the elemental composition change $\xi$ a priori, and therefore, we can actually capture the consequential changes to the $\hat{V}$. In other words, we do not need to know the changes occurring to $\hat{V}$ as a result of changes in the elemental composition a priori, in order to find $\xi$. If we can find the systematic changes to $\hat{V}$ or any physical parameters mentioned earlier without knowing $\xi$, then we do not need IET.

Finally, from Eq. (42), $\ln \hat{V}$ can only be independent of $\xi$ if $\xi \to 0$ or $\xi \to \infty$. Therefore, one can obtain the corresponding $\beta$-functions that satisfy these two limits ($\xi \to 0$ and $\xi \to \infty$) as given below,

$$\lim_{\xi \to 0} \beta(\xi_1^*) = \frac{2}{\lambda \mu r} : \text{satisfies Fermi gas},$$

$$\lim_{\xi \to \infty} \beta(\xi_2^*) \to \infty : \text{superinsulator}.$$  

As a consequence, strong electronic correlation is captured by $\beta(\xi > \xi_1^*) > 2/\lambda \mu r$.

### III. DRESSED PHONON AND TOTAL DIELECTRIC CONSTANT

The derivations covered in this section will be the backbone for the derivation of the acoustic and optical branches in the following section, and a further proof for the dressed phonon is given after that. Physically, $\xi$ in Eq. (23) is the energy needed to excite a particular electron to a finite $r$, not necessarily $r \to \infty$. In the early stages of the ionization energy theory, we used the atomic ionization energy ($r \to \infty$) as the input parameter to compute carrier concentration [8], and for this reason, $\xi$ was labeled as the ionization energy. Furthermore, Eq. (23) is technically easier to use, for example, since $\xi$ is unique for each atom and using the total energy, $E_0 \pm \xi$ as one of the restrictive condition, we can derive the ionization energy based Fermi-Dirac statistics, which can be applied to solids. The respective distributions for electron and hole are given by [8]

$$f_e(E_0, \xi) = \frac{1}{e^{[(E_0 + \xi) - E_F^{(0)}/k_B T]} + 1}, \quad f_h(E_0, \xi) = \frac{1}{e^{[E_F^{(0)} - (E_0 - \xi)]/k_B T} + 1},$$

(45)
where $k_B$ is the Boltzmann constant. The dressed phonon frequency is given by

$$\omega(k)^2 = \frac{\Omega_p^2}{\epsilon(0,k)}; \quad \epsilon(0,k) = 1 + \frac{K_s^2}{k^2}$$  \hspace{1cm} (46)

where $\Omega_p$ is the plasma frequency and $K_s^2 = 3n_0e^2/2\epsilon_0E_F^0$. Here, $E_F^0$ is the Fermi level at $T = 0$, and $K_s$ are the wavenumber and Thomas-Fermi wavenumber, respectively \cite{7}. While, $n_0$ denotes the carrier density (free-electrons) at $T = 0$. The electronic dielectric constant based on the Thomas-Fermi approximation and ionization energy is given by \cite{7}

$$\epsilon(0, \xi, k) = 1 + \frac{K_s^2}{k^2} \exp[\lambda(E_F^0 - \xi)].$$  \hspace{1cm} (47)

Using Eq. (47) and taking $(K_s^2/k^2) \exp[\lambda(E_F^0 - \xi)] \gg 1$, we can rewrite Eq. (46) as

$$\omega(\xi, k) = \frac{k\Omega_p}{K_s} \exp\left[\frac{1}{2}\lambda(\xi - E_F^0)\right],$$  \hspace{1cm} (48)

On the other hand, the constant of proportionality ($\epsilon$) that relates the Fourier transform of the total potential ($\phi$) in a metal to the Fourier transform of the external-charge potential ($\phi_{\text{ext}}$) can be written as

$$\phi = \frac{1}{\epsilon} \phi_{\text{ext}} = \frac{1}{\epsilon_{\text{dressed}}^\text{ion}} \frac{1}{\epsilon_{\text{el}}} \phi_{\text{ext}},$$  \hspace{1cm} (49)

where, $\epsilon$ is defined as the total dielectric constant, $\epsilon(0, k)$. The ionic dressed dielectric constant, $\epsilon_{\text{dressed}}^\text{ion}$ represents the screened ions due to screening electrons. We can rewrite Eq. (49), after taking $(K_s^2/k^2) \exp[\lambda(E_F^0 - \xi)] \gg 1$ and using Eq. (47)

$$\phi = \frac{1}{\epsilon} \phi_{\text{ext}} = \frac{1}{\epsilon_{\text{dressed}}^\text{ion}} \frac{1}{\epsilon_{\text{el}}} \phi_{\text{ext}} \exp[\lambda(E_F^0 - \xi)],$$  \hspace{1cm} (50)

In the presence of electronic medium with ionic medium as an external source, the potentials from the ionic ($\phi_{\text{ion}}$) and the ionic induced electronic ($\phi_{\text{ext}}$) contributions can be written as [using Eq. (47)]

$$\epsilon_{\text{el}} \phi = \phi_{\text{ion}} + \phi_{\text{ext}},$$  \hspace{1cm} (51)

Similarly, considering bare ions with electronic medium as an external source, we can write \cite{9}

$$\epsilon_{\text{ion}}^\text{bare} \phi = \phi_{\text{el}} + \phi_{\text{ext}},$$  \hspace{1cm} (52)

Noting that $\phi = \phi_{\text{el}} + \phi_{\text{ext}} + \phi_{\text{ion}}$, and from Eqs. (17), (19), (21) and (22), we can arrive at

$$\epsilon_{\text{ion}}^\text{dressed} = 1 + \frac{\epsilon_{\text{ion}}^\text{bare} - 1}{1 + (K_s^2/k^2) \exp[\lambda(E_F^0 - \xi)]},$$  \hspace{1cm} (53)

If we take \cite{9} the $\epsilon_{\text{ion}}^\text{bare} = 1 - (\Omega_p^2/w^2)$, then it is straightforward to show that

$$\frac{1}{\epsilon} = \left(\frac{1}{1 + (K_s^2/k^2) \exp[\lambda(E_F^0 - \xi)]}\right) \left(\frac{w^2}{w^2 - w(k)^2}\right),$$  \hspace{1cm} (54)

Equations (53) and (54) suggest that in order to evaluate the changes of the strongly correlated electronic properties with different doping elements, Eq. (17) is sufficient. In this case, the electron-phonon interaction enters through the heavier effective mass \cite{11}. However, phonons cannot be treated as a mere variation to the effective mass if we are interested in thermal properties of correlated matter.
IV. DRESSED ACOUSTIC AND OPTICAL BRANCHES

We consider a 1D lattice with a basis with two different ions per primitive cell and in this system of diatomic linear chain, the harmonic potential energy can be written as:

\[ U_{\text{harm}} = \frac{Q}{2} \sum_n [u_1(na) - u_2(na)]^2 + \frac{G}{2} \sum_n [u_2(na) - u_1((n+1)a)]^2, \]  

where \( u_1(na) \) is the displacement of the first ion that oscillates about the site \( na \), while for the second ion, the displacement is \( u_2(na) \) that oscillates about \( na + d \). Harmonic oscillation requires \( d \leq a/2 \). Using Eq. (50) we can write the interaction potential constants, \( Q \) and \( G \) as:

\[ Q = \frac{\partial^2 \phi(na)}{\partial x^2} \exp[\lambda(\xi - E_F^0)], \]

\[ G = \frac{\partial^2 \phi(na + d)}{\partial x^2} \exp[\lambda(\xi - E_F^0)]. \]

Here, \( \xi \) is the average ionization energy in the vicinity of ionic mass 1 \( (M_1) \) and 2 \( (M_2) \). \( \phi(na) \) and \( \phi(na + d) \) represent the interaction energies between the respective ions through the screening electrons. The exponential term originates from our dressed electron described earlier. The equation of motion based on Eq. (55) can be readily solved to obtain:

\[ \omega_{\pm}^2 = \frac{1}{2M_1M_2} \left[ (Q + G)(M_1 + M_2) \pm \left\{ [(Q + G)^2 \right. \\
\left. \times (M_1 + M_2)^2 - 4M_1M_2((Q + G)^2 - Q^2 - G^2 \\
\left. - 2QG \cos(ka))^1/2 \right] \right \} e^{\lambda(\xi - E_F^0)}. \]

It is clear here that the ionization-energy dress that appears in Eq. (58) is identical with Eq. (48). In the limit \( \xi \to \infty \), then the above system is infinitely rigid. In view of Eq. (48) and (58), we can readily derive (following the procedure described in Ref. [9]) the 1D harmonic oscillator Hamiltonian (in the second quantized form) and its eigenvalues, respectively as:

\[ \hat{H} = \sum_k \hbar \omega(k) e^{\frac{1}{2} \lambda(\xi - E_F^0)} \left[ a_k^\dagger a_k + \frac{1}{2} \right]. \]

\[ E = \sum_k \hbar \omega(k) e^{\frac{1}{2} \lambda(\xi - E_F^0)} \left[ n_k + \frac{1}{2} \right]. \]

Note here that \( n_k \) is the dressed phonon distribution function. The \( a_k^\dagger \) and \( a_k \) denote the usual phonon creation and annihilation operators.

V. DRESSED ELECTRON-PHONON INTERACTION

In the previous sections, what we have done is that we have stripped the ionization-energy dress (exponential term) from the electrons and put it on the phonons (dressed phonon). This implies that we can readily tack the exponential term to the phonon frequency and derive the Debye model and heat capacity. But before we move on, we need to prove that such discriminative dressing (stripping the electrons in order to dress the phonons) is mathematically and theoretically valid. We can prove this by showing that when we tack the exponential term (ionization-energy dress) onto the phonon frequency, we will find that the form appears in the derived dressed \( e-ph \) interaction potential is exactly the same as the form, appeared in the dressed electron-electron (\( e-e \)) screened Coulomb potential (given below) [7].
Using Landau approach [9], we can derive the ionization energy of the effective mass. Consequently, we need to impose this condition of heavier effective mass into Eq. (65). Here, we will make use of the perturbation potential has the electron-phonon interaction effect taken into account implicitly that gives rise to heavier effective mass. This means that for heavier effective mass, we need to satisfy, \[ E_{\perp} = \sum_{n \neq m} \frac{\left| \langle \varphi_m | H_{\text{per}} | \varphi_n \rangle \right|^2}{E_n - E_m} \] (62)

where \( E^{(2)} \) is the second order correction to \( E^{(0)} \). The \( \varphi_{m,n} \) denotes wavefunction for states \( m \) and \( n \), respectively, while \( H_{\text{per}} \) is the perturbation. If we take \( H_{\text{per}} \) as the \( e\text{-}\text{ph} \) interaction potential, \( H_{\text{ep}} \) for solids in \( \mathbf{k} \)-space, and using Eq. (48) then we can rewrite Eq. (62)

\[ E^{(2)} = \sum_{\mathbf{k},\mathbf{k}'} \frac{|\langle \varphi_{\mathbf{k}'} | H_{\text{ep}} | \varphi_{\mathbf{k}} \rangle|^2}{E(\mathbf{k}) - E(\mathbf{k'}) - \hbar \omega(\mathbf{k} - \mathbf{k'}) e^{\frac{i}{\hbar} \lambda (\xi - E_{\mathbf{k}}^0)}} \]

\[ = \sum_{\mathbf{k},\mathbf{k}'} n_{\mathbf{k}}(1 - n_{\mathbf{k}'}) \left[ \frac{|\langle \varphi_{\mathbf{k}'} | H_{\text{ep}} | \varphi_{\mathbf{k}} \rangle|^2}{E(\mathbf{k}) - E(\mathbf{k'}) - \hbar \omega(\mathbf{k} - \mathbf{k'}) e^{\frac{i}{\hbar} \lambda (\xi - E_{\mathbf{k}}^0)}} \right]. \] (63)

The detailed reasons why Eq. (62) represents the \( e\text{-}\text{ph} \) interaction and the missing first-order correction (its matrix elements equal zero due to orthogonality) are given in Ref. [10]. The dressed phonon distribution function can be written as

\[ n_{\mathbf{k}} = \frac{1}{e^{\beta \omega(\mathbf{k}) e^{\frac{i}{\hbar} \lambda (\xi - E_{\mathbf{k}}^0)}} - 1. \] (64)

The denominator in Eq. (63) have made use of the crystal momentum conservation, \( \mathbf{k} - \mathbf{k'} = \mathbf{q} \), and \( \beta = 1/k_B T \). Using Landau approach [9], we can derive the \( e\text{-}\text{ph} \) interaction potential, \( V_{\mathbf{k},\mathbf{k}'} \) from Eq. (58)

\[ V_{\mathbf{k},\mathbf{k}'} = \frac{\partial^2 E^{(2)}}{\partial n_{\mathbf{k}} \partial n_{\mathbf{k}'}} = |g_{\mathbf{k},\mathbf{k}'}|^2 \left[ \frac{2 \hbar \omega(\mathbf{k} - \mathbf{k'}) e^{\frac{i}{\hbar} \lambda (\xi - E_{\mathbf{k}}^0)}}{[\hbar \omega(\mathbf{k} - \mathbf{k'}) e^{\frac{i}{\hbar} \lambda (\xi - E_{\mathbf{k}}^0)}]^2 - [E(\mathbf{k}) - E(\mathbf{k'})]^2} \right]. \] (65)

The \( e\text{-}\text{ph} \) coupling constant, \( |g_{\mathbf{k},\mathbf{k}'}|^2 = |\langle \varphi_{\mathbf{k}'} | H_{\text{ep}} | \varphi_{\mathbf{k}} \rangle|^2 \) is given by [3]

\[ |g_{\mathbf{k},\mathbf{k}'}|^2 = \frac{1}{V e_0} \left[ \frac{e^2}{|\mathbf{k} - \mathbf{k'}|^2 + K^2_\alpha} \right] \frac{1}{2} \hbar \omega(\mathbf{k} - \mathbf{k'}). \] (66)

In the previous work [11], we have claimed that the ionization energy dressed electron-electron screened Coulomb potential has the electron-phonon interaction effect taken into account implicitly that gives rise to heavier effective mass. Consequently, we need to impose this condition of heavier effective mass into Eq. (65). Here, we will make use of the effective mass \( (m^*) \) theorem [3], in which it is approximately given by

\[ \frac{\partial^2 E_n(\mathbf{k})}{\partial \mathbf{k}_i \partial \mathbf{k}_j} \propto \frac{1}{m^*} \delta_{ij} + O \left( \frac{1}{m^*} \right)^2. \] (67)

This means that for heavier effective mass, we need to satisfy, \( \hbar \omega(\mathbf{k} - \mathbf{k'}) e^{\frac{i}{\hbar} \lambda (\xi - E_{\mathbf{k}}^0)} \gg |E(\mathbf{k}) - E(\mathbf{k'})|^2 \). In other words, we need the term, \( |E(\mathbf{k}) - E(\mathbf{k'})|^2 \) to be relatively small in order to comply with Eq. (67), which gives rise to the heavier effective mass effect. As such, Eq. (65) can now be rewritten as (also, after dressing Eq. (66) with the ionization energy)

\[ V_{\text{ep}}(\mathbf{k}, \mathbf{k'}) = \frac{1}{V e_0} \left[ \frac{e^2}{|\mathbf{k} - \mathbf{k'}|^2 + K^2_\alpha \exp[\lambda (E_{\mathbf{k}}^0 - \xi)]} \right]. \] (68)

As anticipated, Eq. (68) is in exact form with Eq. (61). This completes the proof that the ionization energy is proportional to the electron-phonon coupling constant and its relationship with heavier effective mass, where we have only explained this proportionality qualitatively in Ref. [11]. The next step is to apply the outcome of this proof to derive the heat capacity and the well known Debye model (Debye frequency and temperature).
VI. DRESSED HEAT CAPACITY AND DEBYE TEMPERATURE

Now, we will make use of all the results derived earlier to derive the dressed heat capacity formula, dressed Debye frequency and the dressed Debye temperature. The energy density of a harmonic crystal is given by (using Eq. (60) and introducing the static potential energy constant)

$$U = U_{\text{stat}} + \frac{1}{V} \sum_{k,s} \frac{1}{2} \hbar \omega_s(k) e^{\frac{1}{2} \lambda (\xi - E_F^p)} + \frac{1}{V} \sum_{k,s} \frac{\hbar \omega_s(k) e^{\frac{1}{2} \lambda (\xi - E_F^p)}}{e^{\beta \hbar \omega_s(k) e^{\frac{1}{2} \lambda (\xi - E_F^p)}} - 1},$$

(69)

and the non-constant heat capacity ($C_v$) is given by

$$C_v = \frac{\partial U}{\partial T} = \frac{1}{V} \sum_{k,s} \frac{\partial}{\partial T} \frac{\hbar \omega_s(k) e^{\frac{1}{2} \lambda (\xi - E_F^p)}}{e^{\beta \hbar \omega_s(k) e^{\frac{1}{2} \lambda (\xi - E_F^p)}} - 1}. $$

(70)

We also have introduced the branch index, $s = 1,...,3p$, where $p$ is the number of ions in the basis signifying that for each $k$ there are $3p$ normal modes [9]. In the limit of long wavelength (small $k$), \( \omega(k) = c_s(k)k e^{\frac{1}{2} \lambda (\xi - E_F^p)} \) [using Eq. (68)] where $c_s$ is the long wavelength phase velocity that depends on the vibrational polarization, $s$ and the direction of $k$ [9]. Again, using the same procedure given in Ref. [9], we solve Eq. (70) and obtain

$$C_v = \frac{2\pi^2 k_B}{5} \left[ \frac{k_B T}{\hbar c} \right]^3 e^{-\frac{\lambda}{2} (\xi - E_F^p)},$$

(71)

where $k_B$ is the Boltzmann constant and note here that Eq. (71) correctly gives the inverse proportionality between $C_v$ and the ionization energy, $\xi$. Later, this proportionality will be associated to the stiffness of the crystal, as we can anticipate from this relationship itself.

Next, let us work within Debye’s approach and derive the Debye frequency, temperature and the heat capacity, all dressed with ionization energy. In this case, we may simply write,

$$\omega = ck e^{\frac{1}{2} \lambda (\xi - E_F^0)}, \quad k = \frac{\omega}{c} e^{-\frac{1}{2} \lambda (\xi - E_F^0)},$$

(72)

where $c$ is the constant sound velocity. The phonon density of states, $N(\omega)$ is given by

$$N(\omega) = \frac{dN}{d\omega} = \frac{d}{d\omega} \left[ \frac{V \omega^3}{6\pi^2 e^3} e^{-\frac{4}{3} \lambda (\xi - E_F^0)} \right] = \frac{\omega^2 V}{2\pi^2 e^3} e^{-\frac{4}{3} \lambda (\xi - E_F^0)},$$

(73)

where $N$ is the number of phonons. By defining $\omega = \omega_D$ and $n_{ph} = N/V$ as phonon density, we can rewrite Eq. (73) to obtain the Debye frequency

$$\omega_D = c[6\pi^2 n_{ph}]^{1/3} e^{\frac{1}{2} \lambda (\xi - E_F^0)}.$$

(74)

Also noting that $N/V = [k_D e^{-\frac{1}{2} \lambda (\xi - E_F^0)}]^{3/6\pi^2}$ and $k_B \Theta_D = \hbar \omega_D = \hbar c k_D$, then we can arrive at the Debye temperature

$$\Theta_D = \frac{\hbar c}{k_B [6\pi^2 n_{ph}]^{1/3} e^{\frac{1}{2} \lambda (\xi - E_F^0)}}.$$

(75)

Before we continue, it is important to reduce the level of confusion that may arise in the above formulations and proofs with the exponential term appearing here and there. Hence, we will give a step-by-step derivation for the Debye heat capacity, which will prove the origin of the exponential term in Eq. (75), as well as points out the correct way of handling this exponential term. Again, we start from Eq. (70) using \[ dk = k^2 dk d\Omega \] to get \( (\Omega \) is the phonon polarization volume in $k$-space)
\[ C_v = \frac{3\hbar c^2}{2\pi^2 k_B T^2} \int_0^{k_D} k^4 \, dk \, e^{\alpha_k^\beta_L (\xi - E_F^0)} \frac{e^{\beta \hbar c e^\lambda (\xi - E_F^0)}}{[e^{\beta \hbar c e^\lambda (\xi - E_F^0)} - 1]^2} \]  

(76)

Now we make the substitution, \( x = \beta \hbar c e^\lambda (\xi - E_F^0) \) into Eq. (76) and obtain

\[ C_v = 9k_B n_{ph} \left[ \frac{T}{\Theta D e^{\lambda (\xi - E_F^0)}} \right] \int_0^{\infty} \frac{x^4 e^x}{(e^x - 1)^2} \, dx. \]  

(77)

We can see that Eq. (77) is in agreement with Eq. (71) and (75).

VII. CONCLUSIONS

In conclusion, we have proved that the ionization energy theory is indeed a renormalized theory based on the approach developed by Zinn-Justin, Shankar and Gell-Mann–Low formalism. Subsequently, we have applied these proofs to show that the ionization-energy dressed electron-phonon interaction potential is exactly in the same form as the ionization-energy dressed electron-electron Coulomb potential. Consequently, we can obtain the heat capacity and the Debye frequency as a function of ionization energy. These latter proofs can be used to explain the evolution of the electron-phonon interaction with respect to elemental composition in strongly correlated matter. Apart from that, this theory may define the existence of the (quantum) phase transition between free-electron metals and strongly correlated matter, which will be addressed in our future work.

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VIII. APPENDIX

A. Reversible transformation between Eq. (46) and (48)

One should not assume that Eq. (46) and Eq. (48) are not identical or theoretically different. Equations (46) and Eq. (48) are both mathematically and theoretically exact, which can be transformed and reverse-transformed exactly. We have to prove this transformation because obtaining Eq. (48) from Eq. (46) is our starting axiom for the later proofs in this appendix. Hence, by taking the appropriate limits,

\[ \lim_{\xi > E_F^0} \epsilon(0, \xi, k) = 1 + \frac{K_s^2}{k^2} \exp[\lambda(E_F^0 - \xi)]. \]

\[ \lim_{\xi \to E_F^0} \epsilon(0, \xi, k) = 1 + \frac{K_s^2}{k^2} = \epsilon(0, k). \]

and also after taking, \( (K_s^2/k^2) \exp[\lambda(E_F^0 - \xi)] \gg 1 \) and \( K_s^2/k^2 \gg 1 \), we obtain

\[ \lim_{\xi > E_F^0} \omega(\xi, k) = \frac{k\Omega_p}{K_s} \exp \left[ \frac{1}{2} \lambda(\xi - E_F^0) \right], \]

\[ \lim_{\xi \to E_F^0} \omega(\xi, k) = \frac{k\Omega_p}{K_s} = \omega(k) = \frac{\Omega_p}{\sqrt{\epsilon(0, k)}}. \]
For conventional free-electron metals, the \( \lim_{\xi \to E_0^F}^{E_0^F} \) applies and any perturbation due to temperature and/or potential (due to doping, defects, etc.) will vary the \( E_0^F \) and \( n_0 \) accordingly. For example, for each type of free-electron metal, and for each type of perturbation, there are \( n_0 \) and \( E_0^F \), which are both unique. In our approach, any variations to \( E_0^F \) and \( n_0 \) are captured through \( \xi \). Meaning, for a given system, \( E_0^F \) and \( n_0 \) are constants, while \( \xi \) will respond to any perturbations, be it large or small. For example, \( n(r, T, \text{doping}) = n_0 \exp[\lambda(E_0^F - \xi)] \) that will tell us the changes to \( n(r, T, \text{doping}) \). In other words, \( n(r, T, \text{doping}) = n_0(\text{of that perturbed system}), or simply, \( \lim_{\xi \to E_0^F} n(r, T, \text{doping}) = n_0(\text{of that perturbed system}), which will take us back to square one, the free-electron metals [7]. As a consequence, we can see that \( \omega(\xi, k) = \omega(k) \) or Eq. (46) and Eq. (48) are exactly the same due to our reversible transformation.

**B. Derivation of Eq. (54)**

We start from the definition as given in Eq. (49) where,

\[
\epsilon \phi = \phi_{\text{ext}}. \tag{78}
\]

Next, we add Eq. (51) and Eq. (52) to obtain,

\[
\phi(\epsilon_{\text{el}} + \epsilon_{\text{bare}}) = 2\phi_{\text{ext}} + \phi_{\text{ion}} + \phi_{\text{el}}. \tag{79}
\]

We then subtract Eq. (78) from Eq. (79) to get

\[
\phi(\epsilon_{\text{el}} + \epsilon_{\text{bare}} - \epsilon) = \phi_{\text{ext}} + \phi_{\text{ion}} + \phi_{\text{el}}. \tag{80}
\]

Since, \( \phi = \phi_{\text{ext}} + \phi_{\text{ion}} + \phi_{\text{el}} \), Eq. (80) needs to satisfy

\[
\epsilon = \epsilon_{\text{el}} + \epsilon_{\text{bare}} - 1. \tag{81}
\]

Now, if the electrons screen the dressed ions, then Eq. (78) can also be written as

\[
(\epsilon_{\text{ion}}^{\text{dressed}} \epsilon_{\text{el}}) \phi = \phi_{\text{ext}}, \tag{82}
\]

such that [from Eq. (82) and Eq. (81)]

\[
\epsilon_{\text{ion}}^{\text{dressed}} \epsilon_{\text{el}} = \epsilon_{\text{el}} + \epsilon_{\text{ion}}^{\text{bare}} - 1 = \epsilon. \tag{83}
\]

Therefore,

\[
\epsilon_{\text{ion}}^{\text{dressed}} = 1 + \frac{\epsilon_{\text{ion}}^{\text{bare}} - 1}{\epsilon_{\text{el}}}. \tag{84}
\]

Substituting Eq. (77) into Eq. (84) will lead us directly to Eq. (63). Subsequently, we substitute \( \epsilon_{\text{ion}}^{\text{bare}} = 1 - (\Omega_p^2/\omega^2) \) and Eq. (18) into Eq. (84) so as to arrive at

\[
\epsilon_{\text{ion}}^{\text{dressed}} = 1 + \frac{1 - (\Omega_p^2/\omega^2) - 1}{\epsilon_{\text{el}}} = 1 + \frac{(\Omega_p^2 / \omega^2)}{\epsilon_{\text{el}}} = 1 - \frac{\omega(k^2)}{\omega^2}. \tag{85}
\]
From Eq. (83), we can rewrite the total dielectric, $\epsilon$ as

$$
\frac{1}{\epsilon} = \frac{1}{\epsilon_{\text{ion}}} \frac{1}{\epsilon_{\text{dressed}}},
$$

(86)

Substituting Eqs. (85) and (47) into Eq. (86) will lead us to Eq. (54) as shown below,

$$
\frac{1}{\epsilon} = \frac{1}{1 - \left(\frac{\omega}{(k^2/\omega^2)}\right)} \frac{1}{\left(1 + \left(K^2_s/2k^2\right) \exp\left[\lambda(E_0^0 - \xi)\right]\right)}
\frac{1}{w^2 - w(k^2)}.
$$

(87)

C. Derivation of Eq. (58)

Using Eq. (55), the equations of motion can be written as

$$
M_1 \ddot{u}_1(na) = -\frac{\partial U_{\text{harm}}}{\partial u_1(na)} = -\frac{Q}{2} \cdot 2[u_1(na) - u_2(na)] - \frac{G}{2} \cdot 2[u_2(na) - u_1((n+1)a)]
$$

$$
= -Q[u_1(na) - u_2(na)] - G[u_2(na) - u_1((n+1)a)],
$$

(88)

$$
M_2 \ddot{u}_2(na) = -\frac{\partial U_{\text{harm}}}{\partial u_2(na)} = -\frac{Q}{2} \cdot 2[u_1(na) - u_2(na)](-1) - \frac{G}{2} \cdot 2[u_2(na) - u_1((n+1)a)]
$$

$$
= -Q[u_2(na) - u_1(na)] - G[u_2(na) - u_1((n+1)a)].
$$

(89)

The dressed harmonic potential energy ($\phi_{\text{dressed}}(x)$) and the interaction potential constants (Q and G) are respectively, given by

$$
\phi_{\text{dressed}}(x) = \phi(x) \exp[\lambda(\xi - E_0^0)],
$$

(90)

$$
Q_{\text{dressed}} = \frac{\partial^2 \phi_{\text{dressed}}[(na), x]}{\partial x^2} = Q \exp[\lambda(\xi - E_0^0)],
$$

(91)

$$
G_{\text{dressed}} = \frac{\partial^2 \phi_{\text{dressed}}[(na + d), x]}{\partial x^2} = G \exp[\lambda(\xi - E_0^0)].
$$

(92)

Here, the two ions with their respective masses, $M_1$ and $M_2$ have been considered, in which the ionic oscillations are harmonic ($d \leq a/2$). The solutions we need are in the form of

$$
u_1(na) = b_1 e^{i(nk - \omega t)}, \quad u_2(na) = b_2 e^{i(nk - \omega t)},
$$

(93)

where $k$ is the wavevector, while $b_1$ and $b_2$ are constants. By substituting Eq. (93) into Eq. (58) and (59), one can obtain two coupled equations:

$$
[M_1\omega^2 - (Q + G)e^{\lambda(\xi - E_0^0)}]b_1 + [Q + Ge^{i(nk - \omega t)}]b_2 e^{\lambda(\xi - E_0^0)} = 0,
$$

(94)
Due to phonon absorption is given by

\[ [Q + Ge^{ika}]b_2e^{\lambda(\xi - E_0^p)} + [M_2\omega^2 - (Q + G)e^{\lambda(\xi - E_0^p)}]b_1 = 0. \] (95)

These homogeneous equations can be solved by setting the determinant equals zero, i.e.,

\[ [M_1\omega^2 - (Q + G)e^{\lambda(\xi - E_0^p)}][M_2\omega^2 - (Q + G)e^{\lambda(\xi - E_0^p)}] = [(Q + Ge^{ika})b_2e^{\lambda(\xi - E_0^p)}]^2. \] (96)

Therefore,

\[ [M_1M_2]\omega^4 + [-(Q + G)(M_1 + M_2)e^{\lambda(\xi - E_0^p)}]\omega^2 + [(Q + G)^2 - Q^2 - G^2 - 2QG\cos(ka)]e^{2\lambda(\xi - E_0^p)} = 0. \] (97)

By identifying \( A = M_1M_2, \) \( B = -(Q + G)(M_1 + M_2)e^{\lambda(\xi - E_0^p)} \) and \( C = (Q + G)^2 - Q^2 - G^2 - 2QG\cos(ka)]e^{2\lambda(\xi - E_0^p)}, \) we can obtain Eq. (95) from Eq. (98) given below:

\[ \omega^2 = \frac{B \pm \sqrt{B^2 - 4AC}}{2A}. \] (98)

D. Derivation of Eq. (98)

From Eq. (92), \( E_n^{(0)} \) and \( E_m^{(0)} \) are the zeroth order initial and excited states, respectively. As such, their difference due to phonon absorption is given by

\[ E_n^{(0)} - E_m^{(0)} = E(k^*) + \hbar\omega(k - k^*) - E(k). \] (99)

Prior to phonon absorption, one can identify the excited states as unoccupied, while the initial states as occupied, thus, we need to include a probability factor in the form of \( \sum_{k,k^*} n_k(1 - n_{k^*}) \), which satisfies the Bose-Einstein statistics. As a consequence, we can arrive at Eq. (93). The next step is to obtain Eq. (95):

\[ V_{k,k^*} = \frac{\partial^2 E^{(2)}}{\partial n_k \partial n_{k^*}} = \frac{\partial^2}{\partial n_k \partial n_{k^*}} \sum_{k,k^*} n_k(1 - n_{k^*}) \left| \langle \varphi_k | H_{\text{ep}} | \varphi_{k^*} \rangle \right|^2 \]

\[ = |g_{k,k^*}|^2 \left[ \frac{n_k(1 - n_{k^*})}{E(k) - E(k^*) - \hbar\omega(k - k^*)} + \frac{n_{k^*}(1 - n_k)}{E(k^*) - E(k) - \hbar\omega(k^* - k)} \right] \]

\[ = |g_{k,k^*}|^2 \left[ \frac{1}{E(k) - E(k^*) - \hbar\omega(k - k^*)} + \frac{1}{E(k^*) - E(k) - \hbar\omega(k^* - k)} \right] \]

\[ = |g_{k,k^*}|^2 \left[ \frac{2\hbar\omega(k - k^*)e^{\lambda(\xi - E_0^p)}}{[\hbar\omega(k - k^*)e^{\lambda(\xi - E_0^p)}]^2 - [E(k) - E(k^*)]^2} \right], \] (100)

where \( |g_{k,k^*}|^2 = |g_{k^*,k}|^2 \). After dressing Eq. (100) with ionization energy, one obtains

\[ |g_{k,k^*}|^2 = \frac{1}{V_{\text{el}}} \left[ |k - k^*|^2 + K^2e^{\lambda(\xi - E_0^p)} \right] \frac{1}{2} \hbar\omega(k - k^*)e^{\lambda(\xi - E_0^p)}. \] (101)

Substituting Eq. (101) into Eq. (100) leads to
Next, we substitute these equations given below into Eq. (105):

\[
V_{ep}(k, k^*) = \frac{e^2}{2V\epsilon_0} \frac{\hbar \omega(k - k') e^{\frac{1}{2}\lambda(\xi - E_F^0)} [2\hbar \omega(k - k') e^{\frac{1}{2}\lambda(\xi - E_F^0)} - [E(k) - E(k^*)]^2]}{|k - k'|^2 + K_s^2 e^{\lambda(\xi - E_F^0)}]}
\]

(102)

Now, invoking the effective mass theorem [Eq. (67)], Eq. (102) can be written as given below to obtain Eq. (68).

\[
V_{ep}(k, k^*) = \frac{e^2}{2V\epsilon_0} \frac{\hbar \omega(k - k') e^{\frac{1}{2}\lambda(\xi - E_F^0)} [2\hbar \omega(k - k') e^{\frac{1}{2}\lambda(\xi - E_F^0)} - [E(k) - E(k^*)]^2]}{|k - k'|^2 + K_s e^{\lambda(\xi - E_F^0)}]}
\]

(103)

E. Derivation of Eq. (71)

Equation (60) can also be written as

\[
U = U_{stat} + \frac{1}{V} \sum_{k,s} \frac{1}{2} \hbar \omega_s(k) e^{\frac{1}{2}\lambda(\xi - E_F^0)} + \frac{1}{V} \sum_{k,s} \hbar \omega_s(k) e^{\frac{1}{2}\lambda(\xi - E_F^0)} n_k,
\]

(104)

After substituting Eq. (64) into Eq. (104), one can arrive at Eq. (69). Whereas, the \(C_v\) can be derived from Eq. (104) as

\[
C_v = \frac{\partial U}{\partial T} = \frac{1}{V} \sum_{k,s} \frac{\partial}{\partial T} \frac{\hbar \omega_s(k) e^{\frac{1}{2}\lambda(\xi - E_F^0)}}{e^{\beta \hbar \omega_s(k) e^{\frac{1}{2}\lambda(\xi - E_F^0)}} - 1}
\]

(105)

Next, we substitute these equations given below into Eq. (106):

\[
\omega(k) = c_s(k) k e^{\frac{1}{2}\lambda(\xi - E_F^0)}, \quad dk = k^2 dk \quad \sin \theta \, d\theta \, d\phi = k^2 dk d\Omega,
\]

(106)

\[
x = \frac{\beta \hbar c_s e^{\frac{1}{2}\lambda(\xi - E_F^0)}}{dk} = \beta \hbar c_s e^{\frac{1}{2}\lambda(\xi - E_F^0)}.
\]

(107)

Hence, we get

\[
C_v = \sum_s \frac{\partial}{\partial T} \int \frac{k^2 dk \, d\Omega}{(2\pi)^3} \frac{\hbar c_s e^{\frac{1}{2}\lambda(\xi - E_F^0)}}{e^{\beta \hbar c_s e^{\frac{1}{2}\lambda(\xi - E_F^0)}} - 1}
\]

(108)

Using
\[ \frac{1}{c^3} = \frac{1}{3} \sum_s \int \frac{d\Omega}{4\pi} \cdot \frac{1}{c^3} \]  

(109)

\[ \int_0^\infty \frac{x^3 dx}{e^x - 1} = \sum_{n=1}^\infty \int_0^\infty x^3 e^{-nx} dx = 6 \sum_{n=1}^\infty \frac{1}{n^4} = \frac{\pi^4}{15}. \]  

(110)

we obtain Eq. (71).

\[ C_v = \frac{\pi^2 k_B}{10} \frac{\partial T^3}{\partial T} \left( \frac{k_B}{\hbar} \right)^3 e^{-\frac{1}{2}\lambda(\xi - E_F^p)} \]

\[ = \frac{2\pi^2 k_B}{5} \left( \frac{k_B T}{\hbar} \right)^3 e^{-\frac{1}{2}\lambda(\xi - E_F^p)}. \]  

(111)

Alternatively, instead of using Eq. (107), we use

\[ x = \beta \hbar c_s k, \quad \frac{dx}{dk} = \beta \hbar c_s, \]  

(112)

to get [also after using Eq. (109)]

\[ C_v = \frac{\partial}{\partial T} \sum_s \int \frac{d\Omega}{4\pi} \int \frac{k^2 dk}{2\pi^2} \frac{h c_s e^{\frac{1}{2}\lambda(\xi - E_F^p)}}{e^{\beta h c_s} \exp \left[ \frac{1}{2}\lambda(\xi - E_F^p) \right] - 1} \]

\[ = \frac{1}{2\pi^2} \frac{\partial}{\partial T} \sum_s \int \frac{d\Omega}{4\pi} \int \left[ \frac{x}{\beta h c_s} \right]^2 \cdot \left[ \frac{dx}{\beta h c_s} \right] \frac{x e^{\frac{1}{2}\lambda(\xi - E_F^p)}}{e^{\beta h c_s} \exp \left[ \frac{1}{2}\lambda(\xi - E_F^p) \right] - 1} \]

\[ = \frac{3}{2\pi^2} \frac{e^{\frac{1}{2}\lambda(\xi - E_F^p)}}{h^3 c_s} \frac{(1/\beta^4)}{\partial(1/\beta^4)} \int_0^\infty \frac{x^3 dx}{e^x \exp \left[ \frac{1}{2}\lambda(\xi - E_F^p) \right] - 1}. \]  

(113)

Substituting

\[ \int_0^\infty \frac{x^3 dx}{e^{x} \exp \left[ \frac{1}{2}\lambda(\xi - E_F^p) \right] - 1} = \sum_{n=1}^\infty \int_0^\infty x^3 \exp \left[ -nx e^{\frac{1}{2}\lambda(\xi - E_F^p)} \right] dx = 3! \left[ \frac{1}{e^{\frac{1}{2}\lambda(\xi - E_F^p)}} \right]^4 \sum_{n=1}^\infty \frac{1}{n^4} \]

\[ = \frac{\pi^4}{15} \frac{1}{e^{2\lambda(\xi - E_F^p)}}, \]  

(114)

into Eq. (113), we can see that Eq. (113) becomes Eq. (111), which is Eq. (71).

F. Derivation of Eq. (75)

From the left-hand side (LHS) equation of Eq. (106),

\[ k = \frac{\omega}{c} e^{-\frac{1}{2}\lambda(\xi - E_F^p)}. \]  

(115)

On the other hand, the number of phonon modes, \( N \) is given by

\[ N = \frac{(4\pi/3)k^3}{(2\pi/L)^3} = \frac{V k^3}{6\pi^2}, \]  

(116)
where $L$ and $V$ are the length and volume, respectively. Next, by substituting Eq. (115) into Eq. (116),

$$N = \frac{V \omega^3}{6\pi^2 c^3} e^{-\frac{2}{3} \lambda (E - E_F^\text{p})},$$

(117)

and differentiating Eq. (117) with respect to $\omega$ will lead us directly to Eq. (73). Substituting Eq. (115) into Eq. (117) gives

$$\frac{N}{V} \frac{\omega^3}{6\pi^2 c^3} = e^{-\frac{2}{3} \lambda (E - E_F^\text{p})} = k^3 e^{-\frac{2}{3} \lambda (E - E_F^\text{p})},$$

$$\frac{N}{V} \frac{\omega^3}{6\pi^2 c^3} = k^3.$$  

(118)

Subsequently, we define, $k = k_D$ and $\omega = \omega_D$, thus

$$k_B \Theta_D = h \omega_D = \hbar k_D, \quad \Theta_D = \frac{\hbar c}{k_B} k_D.$$

(119)

Inserting Eq. (118) into Eq. (119) gives

$$\Theta_D = \frac{\hbar c}{k_B} \left[ \frac{6\pi^2 N e^{\frac{2}{3} \lambda (E - E_F^\text{p})}}{V} \right]^{\frac{1}{3}},$$

(120)

which is equivalent to Eq. (75) by noting that $n_{ph} = N/V$.

### G. Derivation of Eq. (77)

From Eq. (76), noting $\lim_{V \to \infty} (1/V) \sum_k = \int \frac{d\mathbf{k}}{(2\pi)^3}$, and using the RHS equation of Eq. (106) one gets

$$C_v = \frac{3\hbar c}{2\pi^2} \int_{0}^{k_D} k^3 dk e^{\frac{2}{3} \lambda (E - E_F^\text{p})} \frac{\partial}{\partial T} \left[ \frac{1}{e^{\beta h\hbar c e^{\frac{2}{3} \lambda (E - E_F^\text{p})}} - 1} - 1 \right],$$

(121)

where

$$c = \left[ \frac{1}{3} \sum_s \int \frac{d\Omega}{4\pi} C_s(k) \right]_{\text{isotropic}} \left( \text{polarization} \right),$$

(122)

$$\frac{\partial}{\partial T} \left[ \frac{1}{e^{\beta h\hbar c e^{\frac{2}{3} \lambda (E - E_F^\text{p})}} - 1} - 1 \right] = \frac{\partial}{\partial T} \left[ e^{\beta h\hbar c e^{\frac{2}{3} \lambda (E - E_F^\text{p})}} - 1 \right]^{-1} = -1 [e^{\beta h\hbar c e^{\frac{2}{3} \lambda (E - E_F^\text{p})}} - 1]^{-2} \left[ -\frac{\hbar c k}{k_B T^2} e^{\beta h\hbar c e^{\frac{2}{3} \lambda (E - E_F^\text{p})}} \right]$$

$$= \frac{\hbar c k}{k_B T^2} \left[ e^{\beta h\hbar c e^{\frac{2}{3} \lambda (E - E_F^\text{p})}} - 1 \right]^{-2},$$

(123)

Therefore, we can derive $C_v$ as given in Eq. (77). Consequently, after the change of variables as given in Eqs. (106) and (107),

$$C_v = \frac{3(\hbar c)^2}{2\pi^2 k_B T^2} \int_{0}^{k_D} k^4 dk e^{\frac{2}{3} \lambda (E - E_F^\text{p})} \left[ e^{\beta h\hbar c e^{\frac{2}{3} \lambda (E - E_F^\text{p})}} - 1 \right]^2$$

$$= \frac{3(\hbar c)^2}{2\pi^2 k_B T^2} \int_{0}^{k_B T} \frac{d\mathbf{k}_B T}{(\hbar c)^2 e^{2\lambda (E - E_F^\text{p})}} \frac{dx k_B T}{\hbar c e^{\frac{2}{3} \lambda (E - E_F^\text{p})}} \left[ e^{\beta h\hbar c e^{\frac{2}{3} \lambda (E - E_F^\text{p})}} - 1 \right]^2$$

$$= \frac{3(\hbar c)^2}{2\pi^2 k_B T^2} \left[ \frac{k_B T}{\hbar c} \right]^5 e^{(1 - 2 - \frac{1}{3}) \lambda (E - E_F^\text{p})} \int_{0}^{\infty} \frac{x^4 e^x dx}{(e^x - 1)^2}. $$

(124)
From Eq. (119), one gets $hc = (k_B \Theta_D / k_D)$. Substituting this and Eq. (116) into Eq. (124), and after some algebraic rearrangements, one can arrive at

$$C_v = \frac{3(hc)^2}{2\pi^2 k_B T^2} \left[ k_B T \right]^5 e^{(1-2-\frac{1}{3})\lambda (x-E_p^0)} \int_0^{\exp} x^4 e^x dx \left( e^x - 1 \right)^2$$

$$= \frac{3k_B T^3}{2\pi^2 (hc)^3} e^{-\frac{1}{2} \lambda (x-E_p^0)} \int_0^{\exp} x^4 e^x dx \left( e^x - 1 \right)^2$$

$$= \frac{3k_B}{2\pi^2 (6\pi^2 n_{ph})} \left[ T \Theta_D e^{\frac{1}{2} \lambda (x-E_p^0)} \right] \int_0^{\exp} x^4 e^x dx \left( e^x - 1 \right)^2,$$

(125)

which is nothing but Eq. (77). Again, using Eq. (119) and $x_D = \beta \hbar c k_D = (k_B \Theta_D / k_B T) = \Theta_D / T \to \infty$ for $T < \Theta_D$, one can solve Eq. (125):

$$\int_0^{\exp} x^4 e^x dx \left( e^x - 1 \right)^2 = \sum_{n=1}^{\infty} \int_0^{\exp} x^4 e^{n(x-2x)} dx = 4! \sum_{n=1}^{\infty} \frac{1}{n^4} = \frac{24\pi^4}{90},$$

(126)

therefore,

$$C_v = \frac{12\pi^4}{5} n_{ph} k_B \left[ \frac{T}{\Theta_D e^{\frac{1}{2} \lambda (x-E_p^0)}} \right]^3.$$

(127)

If we use Eq. (112) instead, then we need to invoke Eq. (114) and the result [Eq. (127)] remains the same: From Eq. (129)

$$C_v = \frac{3(hc)^2}{2\pi^2 k_B T^2} \int_0^{\exp} k_B dke^{\lambda (x-E_p^0)} e^{\beta \hbar c k_B e^{\frac{1}{2} \lambda (x-E_p^0)}} \left[ e^{\beta \hbar c k_B e^{\frac{1}{2} \lambda (x-E_p^0)}} - 1 \right]^2$$

$$= \frac{3(hc)^2}{2\pi^2 k_B T^2} e^{\lambda (x-E_p^0)} \int_0^{\exp} \left[ \frac{x}{\beta \hbar c} \right]^4 \left[ \frac{dx}{x^4 e^{\lambda (x-E_p^0)}} \right] e^{\frac{1}{2} \lambda (x-E_p^0)}$$

$$= \frac{3k_B T^3}{2\pi^2 (hc)^3} e^{\lambda (x-E_p^0)} \int_0^{\exp} x^4 e^{\frac{1}{2} \lambda (x-E_p^0)} dx.$$

(128)

Using $hc = (k_B \Theta_D / k_D)$ and Eq. (116),

$$C_v = \frac{3}{2\pi^2 n_{ph} 6\pi^2 k_B e^{\lambda (x-E_p^0)} T^3}{\Theta_D^3} \int_0^{\exp} x^4 e^{\frac{1}{2} \lambda (x-E_p^0)} dx.$$

(129)

From,

$$\int_0^{\exp} x^4 dx \left( e^x \left[ \frac{1}{2} \lambda (x-E_p^0) \right] - 1 \right)^2 = \sum_{n=1}^{\infty} \int_0^{\exp} x^4 \exp \left[ n(x-2x)e^{\frac{1}{2} \lambda (x-E_p^0)} \right] dx = 4! \left[ e^{\frac{1}{2} \lambda (x-E_p^0)} \right] ^5 \sum_{n=1}^{\infty} \frac{1}{n^4}$$

$$= \frac{24\pi^4}{90} \frac{1}{e^{\frac{1}{2} \lambda (x-E_p^0)}},$$

(130)

we can rewrite Eq. (129) as

$$C_v = \frac{12\pi^4}{5} n_{ph} k_B e^{(1-\frac{1}{2})\lambda (x-E_p^0)} \left[ \frac{T}{\Theta_D} \right]^3.$$

(131)
which is Eq. \[(127)\].