Discrete and Weyl density of states for photonic dispersion relation

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Abstract
The current density of states (DOS) calculations do not take into account the essential discreteness of the state space, since they rely on the unbounded continuum approximation. Recently, discrete DOS based on the quantum-mechanically allowable minimum-energy interval has been introduced for the quadratic dispersion relation. In this work, we consider systems exhibiting a photonic (photon-like) dispersion relation and calculate the related density and number of states (NOS). Also, a Weyl’s conjecture-based DOS function is calculated for photons and acoustic phonons at a low-frequency limit, by considering the bounded continuum approach. We show that the discrete DOS function reduces to expressions of bounded and unbounded continua in the appropriate limits. The fluctuations in discrete DOS completely disappear under accumulation operators. It is interesting that relative errors of NOS and DOS functions with respect to discrete ones have exactly the same character as the ones of the quadratic dispersion relation. Furthermore, the application of discrete and Weyl DOS for the calculation of internal energy of a photon gas is presented and the importance of discrete DOS is discussed. It is shown that the discrete DOS function given in this work needs to be used whenever the low energy levels of a physical system are heavily occupied.

Keywords: density of states, Weyl’s conjecture, confined systems

(Some figures may appear in colour only in the online journal)

1. Introduction
The density of states (DOS) of a system is an important concept that counts the number of states per interval of energy for each energy level [1]. However, the orthodox calculations of the DOS in general are restricted by the unbounded continuum approximation. Furthermore, the state space is essentially discrete because of the finiteness of the domains and additionally due to the wave character of the particles. This discreteness is however, overlooked by recourse to the argument that the domain sizes of interest are usually much greater than the de Broglie wavelength of the particles. This reasoning naturally allows us to make use of the continuous density of states (CDOS) function prevalent in current literature [2–5]. The recent progress in nano-science and nano-technology indicates that the concept of the density of states is also useful in these cutting edge fields [6–12]. However, it should be noted that domain sizes can often be on the order of the de Broglie wavelength of particles at nano-scale. When this is the case, the bounded continuum approximation is more appropriate to use, since it takes into account the non-zero value of the ground states associated with the momentum components. The bounded continuum approximation forms the ingredient of the Weyl’s conjecture, which sets the stage to understand the behaviour of the eigenvalues asymptotically. Therefore, Weyl’s conjecture provides a more accurate enumeration of the states. This we call the Weyl density of states (WDOS). Despite this improvement though, both
CDOS and WDOS have at their very cores the so-called continuum approximation, and therefore a lack of capturing the feature of essential discreteness.

The discreteness becomes particularly important when quantum confinement cannot be neglected due to the fact that quantum mechanics always implies a quantum confinement in the feature of essential discreteness. Therefore, one should consider this quantum mechanical finiteness of the energy levels and calculate the density of states in a completely discrete manner. Recently, such an approach has been used, contributing to the limited number of studied on the DOS [12–22], to enumerate the number of states exactly by taking into account the discreteness of the minimum allowable energy interval as dictated by quantum mechanics, namely, the discrete density of states function (DDOS) [23]. This approach has been used for the usual, but important, particle in a box model and has been shown to lead to both bounded and unbounded continua expressions in the appropriate limits [23].

The aim of this work is first to calculate the DDOS for photons and acoustic phonons (where the dispersion relation is photon-like) and then compare the findings with those of the usual CDOS and WDOS. We also compare these results with the ones of the quadratic dispersion relation, which actually bears quite a few resemblances. To show the importance of the WDOS and DDOS, the internal energy of a black-body radiation in a confined structure is given as an example. It is seen that the results based on the WDOS match reasonably well with those of the DDOS for weakly and even moderately confined structures (until \( \alpha = 1 \)), while the CDOS is failing for even weakly confined (around \( \alpha = 0.1 \)) structures. For strongly confined (\( \alpha > 1 \)) structures, however, the DDOS may need to be used to get accurate results.

2. D-dimensional forms of DOS functions for photonic dispersion relation

For the particles obeying the photonic dispersion relation confined in a D-dimensional rectangular domain, the dimensionless energy eigenvalues are written as

\[
\tilde{\varepsilon} = \frac{\varepsilon}{k_B T} = \frac{\hbar \omega}{k_B T} = \frac{\hbar v}{2\pi k_B T}|\vec{k}| = L^\alpha \left( \sum_{n=1}^{D} \left( \frac{i_n}{L_n} \right)^2 \right)^{1/2},
\]

where \( k_B \) is Boltzmann’s constant, \( T \) is temperature, \( h \) is the Planck’s constant, \( v \) is the speed of photons or acoustic phonons, \( \vec{k} \) is wave vector, \( D \) is the number of spatial dimensions, \( i_n \) is quantum state variable varying from one to infinity, \( L_n = (hv)/(2\pi k_B T) \) is a characteristic length scale, \( L_n \) is the size of the domain in direction \( n \) and \( \alpha_n = L_n/L_n \) is a confinement parameter in the \( n \)th direction. The calculations of the DOS and NOS functions in this article will be done considering this dispersion. As the DOS functions are used along with distribution functions in statistical mechanics to calculate physical properties of a system, throughout the article, dimensionless energy (\( \tilde{\varepsilon} = \varepsilon/(k_B T) \)) is adopted rather than the energy itself for the compactness of the expressions.

The DDOS function converts multiple summations over discrete quantum states into a single summation over discrete energy states as follows [23]:

\[
\sum_{i_{-1}}^{\infty} \cdots \sum_{i_{D}}^{\infty} f(\tilde{\varepsilon}_i, \cdots, \tilde{\varepsilon}_D) \Delta i_1 \cdots \Delta i_D = \sum_{\tilde{\varepsilon} = \tilde{\varepsilon}_0}^{\infty} f(\tilde{\varepsilon}) DDOS(\tilde{\varepsilon}),
\]

where \( \tilde{\varepsilon}_0 = \sqrt{\alpha_1^2 + \cdots + \alpha_D^2} \) is the ground state energy and \( \Delta \tilde{\varepsilon} \) is the quantum-mechanically minimum-allowed energy difference between successive levels. Note that \( \Delta \tilde{\varepsilon} \) is not a constant quantity unlike \( d\tilde{\varepsilon} \). The analytical solution of \( \Delta \tilde{\varepsilon} \) is only possible for a 1D case so that the numerical calculation of the energy intervals between successive levels requires approximating the energy spectrum data through equation (1) first and then applying the ascending sorting process. This data contains all possible degeneracies inherently, since it is the full energy spectrum. Hence, the definition of the DDOS is given by

\[
DDOS_D(\tilde{\varepsilon}) = \frac{\Delta \Omega_D(\tilde{\varepsilon})}{\Delta \tilde{\varepsilon}} = \frac{\Omega_D(\tilde{\varepsilon} + \Delta \tilde{\varepsilon}) - \Omega_D(\tilde{\varepsilon})}{\Delta \tilde{\varepsilon}},
\]

where \( \Omega_D \) is the discrete number of states (DNOS) given by,

\[
\Omega_D(\tilde{\varepsilon}) = DNOS_D(\tilde{\varepsilon}) = \sum_{i_{-1}}^{\infty} \cdots \sum_{i_{D}}^{\infty} \left[ \Theta(\tilde{\varepsilon} - \sum_{n=1}^{D} (\alpha_n i_n)^2) \right],
\]

where \( \Theta \) is the left-continuous Heaviside step function so that \( \Theta(0) = 0 \).

Considering Weyl’s conjecture in a 3D finite-size domain [1], it is possible to write the WNOs function using the dispersion relation of equation (1) as

\[
WNOS_D(\tilde{\varepsilon}) = \frac{\pi}{6 L^2} \tilde{\varepsilon}^3 \Theta(D - 2) + (-1)^{D-1} \frac{\pi}{4 D-4} S L^2 \tilde{\varepsilon}^2 \Theta(D - 1) + (-1)^{D-2} \frac{P}{4 L^2} \tilde{\varepsilon} \Theta(D),
\]

and from the derivative of the WNOS, we get the WDOS function as

\[
WDOS_D(\tilde{\varepsilon}) = \frac{\pi}{2 L^2} \tilde{\varepsilon}^2 \Theta(D - 2) + (-1)^{D-1} \frac{\pi}{4 D-2} S L^2 \tilde{\varepsilon} \Theta(D - 1) + (-1)^{D-2} \frac{P}{4 L^2} \Theta(D),
\]

where \( V \) is volume, \( S \) is surface area, \( P \) is periphery and \( N_v \) is the number of vertices. These parameters together constitute the geometric size variables of the domain. Note that equations (5) and (6) are not just for rectangular geometries but universal so that they are valid for any confinement geometry. Using equations (5) and (6) neglecting the high-

2
order correction terms (terms having low-dimensional size variables), the CNOS and CDOS functions can be obtained for $D$-dimensional rectangular domain as

\begin{equation}
\text{CNOS}_D(\mathfrak{e}) = \frac{\pi^{D/2} \mathfrak{e}^D L_1 \cdots L_D}{2^D \Gamma((D + 2)/2)L_D},
\end{equation}

\begin{equation}
\text{CDOS}_D(\mathfrak{e}) = \frac{\pi^{D/2} \mathfrak{e}^D L_1 \cdots L_D}{2^{D-1} \Gamma((D + 2)/2)L_D},
\end{equation}

respectively.

The subbands appear for confined directions in the case of lower-dimensional structures. To this aim, $\mathfrak{e}$ variables in the equations of this article need to be modified to $\sqrt{\mathfrak{e}^2 - \mathfrak{e}_{i}^2}$ for lower dimensions and the summation operator $\sum_{\mathfrak{e}} \Theta(\sqrt{\mathfrak{e}^2 - \mathfrak{e}_{i}^2}) \times \cdots$ over subbands must be added to the expressions.

### 2.1. Analytical expressions of WNOS and WDOS functions in various dimensions

Analytical expressions of the WDOS functions are obtained by considering the bounded continuum approximation, which corresponds to the first two terms of Poisson Summation Formula (PSF) [24]. To find the analytical expressions of the WNOS and WDOS functions for the photonic dispersion relation, we first apply the same methodology, based on the first two terms of the PSF, presented in [23] to the DNOS function, equation (4). Note that the derivations for lower-dimensional cases are carried out without considering the subbands of confined directions, so the 2D and 1D treatments are identified as if the actual dimension of the space is not 3D, but lower-dimensional.

By replacing summations in equation (4) by the first two terms of the PSF, WNOS functions for 3D, 2D and 1D cases are obtained, respectively, as

\begin{equation}
\text{WNOS}_3 = \frac{\pi \mathfrak{e}^3}{6 \alpha_1 \alpha_2 \alpha_3} - \frac{\pi \mathfrak{e}^2}{8} \left( \frac{1}{\alpha_1 \alpha_2} + \frac{1}{\alpha_1 \alpha_3} + \frac{1}{\alpha_2 \alpha_3} \right) + \frac{\mathfrak{e}}{4} \left( \frac{1}{\alpha_1} + \frac{1}{\alpha_2} + \frac{1}{\alpha_3} \right) - \frac{1}{8},
\end{equation}

\begin{equation}
\text{WNOS}_2 = \frac{\pi \mathfrak{e}^2}{4 \alpha_1 \alpha_2} - \frac{\mathfrak{e}}{2} \left( \frac{1}{\alpha_1} + \frac{1}{\alpha_2} \right) + \frac{1}{4},
\end{equation}

\begin{equation}
\text{WNOS}_1 = \frac{\mathfrak{e}}{\alpha_1} = \frac{1}{2}.
\end{equation}

The first terms of each equation above gives the corresponding CNOS functions. Straightforward differentiation of the above equation yields

\begin{equation}
\text{WDOS}_3 = \frac{\pi \mathfrak{e}^2}{2 \alpha_1 \alpha_2 \alpha_3} - \frac{\mathfrak{e}^2}{4} \left( \frac{1}{\alpha_1 \alpha_2} + \frac{1}{\alpha_1 \alpha_3} + \frac{1}{\alpha_2 \alpha_3} \right) + \frac{1}{4} \left( \frac{1}{\alpha_1} + \frac{1}{\alpha_2} + \frac{1}{\alpha_3} \right),
\end{equation}

\begin{equation}
\text{WDOS}_2 = \frac{\pi \mathfrak{e}^2}{2 \alpha_1 \alpha_2} - \frac{1}{2} \left( \frac{1}{\alpha_1} + \frac{1}{\alpha_2} \right),
\end{equation}

\begin{equation}
\text{WDOS}_1 = \frac{1}{\alpha_1},
\end{equation}

The first terms of each equation above gives the corresponding CDOS functions. It is appropriate to use the CNOS and CDOS functions only if confinement parameters are much smaller than unity.

It should be noted that exact analytical expression of the DDOS is equal to the WDOS for the 1D case unlike the 2D and 3D cases, since only one state is present in each energy level, i.e. $\Delta \Omega_1 = \Omega_1(\mathfrak{e} + \Delta \mathfrak{e}) - \Omega_1(\mathfrak{e}) = \Delta \mathfrak{e} = 1$. Due to the lack of degeneracy, we simply have $\Delta \mathfrak{e} = \alpha_1$. As a result, the DDOS can analytically be obtained as

\begin{equation}
\text{DDOS}_1 = \frac{\Delta \Omega_1}{\Delta \mathfrak{e}} = \frac{1}{\alpha_1} = \text{WDOS}_1 = \text{CDOS}_1,
\end{equation}

only for the 1D case.

### 3. Results and discussion

#### 3.1. Comparisons of discrete, Weyl and classical DOS and NOS functions

Analytical expressions of the WNOS and WDOS as well as the CNOS and CDOS functions are given without considering subbands. During the calculations of figures for lower-dimensional cases, however, the contributions of subbands are considered by using the modification procedures defined for the related equations in the first paragraph after equation (8). Thus, during the examination of functional behaviors of the DOS and NOS functions, $\mathfrak{e}$ is replaced by $\sqrt{\mathfrak{e}^2 - \mathfrak{e}_{i}^2}$ in all expressions to see the effects of the subbands. In figures 1(a)–(c), equations (3), (10) and (8) are used to draw the DDOS, WDOS and CDOS functions represented by black dots, blue and red curves, respectively. The extremely fluctuating feature of the DDOS is evident in figures 1(a)–(c) when compared with the rather smooth behaviour of the CDOS and WDOS. In this sense, the DDOS is essentially seen to be very different to both the CDOS and WDOS. However, the usual thermodynamic practice almost always includes DOS functions to be smoothed out through a summation or integration process. If this was not the case, it is apparent that the use of the DOS does not yield the same results as the CDOS or WDOS. The transition from this extremely fluctuating behaviour of the DDOS to a rather smooth one can be explicitly observed by inspecting figures 1(d)–(f) and comparing the corresponding DDOS and DNOS plots. In figures 1(d)–(f), equations (4), (9) and (7) are used to draw the DNOS, WNOS and CNOS functions represented by black dots, blue curves and red curves, respectively. Note that the WNOS and CNOS too, are different from one another as can be seen from figures 1(d)–(f), although they both rely on the continuum approximation. The difference lies in the fact that the WNOS makes use of the bounded continuum approximation, whereas the CNOS of the unbounded one. Since the WNOS almost perfectly matches the DNOS, it should be favored to the CNOS as long as confinement is not negligibly weak.
When the DOS and NOS functions given in Figure 1 are compared with the ones given in [23] for the quadratic dispersion relation, it is seen that the dimensional characteristic behaviors changed. For example, the constant-like nature of the 2D DOS function for quadratic dispersion is seen in the 1D DOS here, or square root dependence of the 3D DOS function on energy for quadratic dispersion is seen here in the 2D DOS. Similar change in the functional dependence on energy can also be seen in the NOS functions. Functional energy dependence can easily be predicted from the powers of $\tilde{\epsilon}$ in equations (9) and (10). Although the 1D NOS function seems to have a linear dependency on energy, equation (9c), this dependence only appears in a hypothetical 1D world where all subbands are disappeared. Moreover, in reality 1D behavior appears when the other two directions are strongly confined and constitute subbands. Therefore, due to the existence of subbands, even for the 1D case, non-linear behavior appears at the beginning of each subband since $\tilde{\epsilon}$ is replaced by $\sqrt{\tilde{\epsilon}^2 - \tilde{\epsilon}_s^2}$, Figure 1(f). Moreover, subfigures of Figures 1(d)–(f) shows that errors of the WNOS functions always lower than the CNOS, while errors of both functions increase with decreasing energy near ground state.

The gradual changes of relative errors with increasing confinement and energy as well as with increasing NOS are examined in 3D graphs in Figures 2(a) and (b). It is seen that relative errors oscillate around zero (having both positive and negative values), after starting from very large error values at near ground state energies or low NOS. Increment in confinement shifts the ground state energy to higher energies and grows the magnitude of oscillations. As expected, errors decrease with increasing energy and NOS or decreasing confinement. Relative errors decrease with increasing NOS just like in the quadratic dispersion case. In fact, it is worth emphasizing that relative error results given for the photonic dispersion relation have exactly the same character with those of the quadratic dispersion relation (see [23]). Since the photonic dispersion relation considered in this article is just the square root of the energy in the quadratic one, the relative errors become the same for both dispersions while the DDOS and DNOS functions are different.

3.2. Internal energy of a confined photon gas: comparison of the results based on different DOS functions

From the relative errors of the NOS functions in the previous subsection, it is seen that the WNOS very accurately represents the exact behavior as long as the system is not very close to the ground state. In this subsection, we show the accuracy and limitations of the WDOS function through examining the internal energy of a photon gas that is an important quantity also for the calculation of micro-/nano-scale radiative heat transfer for instance.
The internal energy of a photon gas, confined in a rectangular domain, can be calculated in its dimensionless form as

\[
\frac{U}{k_B T} = p_e \sum_{\ell=1}^{\infty} \sum_{\ell'=1}^{\infty} \sum_{p=1}^{\infty} \mathcal{f}_{\text{BE}}(\xi) \Delta \xi \approx \int \mathcal{f}_{\text{BE}} \text{WDOS}(\xi) d\xi,
\]

where \( p_e \) is the polarization degree of freedom and \( f_{\text{BE}} = \frac{1}{[\exp(\xi) - 1]} \) is the Bose–Einstein distribution function for photons (\( \mu = 0 \)). Equation (12) shows how the DDOS and WDOS can be applied to calculate thermodynamic observables, such as internal energy.

We now calculate the internal energy of a photon gas by using discrete, Weyl and continuous DOS functions. In figure 3, comparisons of internal energy values calculated from DDOS, WDOS and CDOS functions denoted by black, dashed-cyan and orange curves, respectively, are shown for various dimensional isometric and anisometric confinement cases. It is seen that using CDOS functions in internal energy calculations give inaccurate results, especially in case the system is strongly confined at least in one direction (figure 3(d)). On the other hand, internal energy calculated using WDOS functions quite fairly matches the exact results based on the DDOS. However, as is seen from the relative errors of Weyl internal energies (blue curves) in subfigures of figures 3(a)–(d), even using the WDOS gives incorrect results when the confinement is strong enough, though the internal energy itself has relatively small values in this condition. Nevertheless, this condition can appear at very low temperatures or in very small confinement domains.

3.3. Conclusion

To sum up, when the low energy levels are largely occupied as in the cases of low temperature or strong confinement, the DDOS gives better results than even the WDOS. However, since the calculation of DDOS requires more computational efforts than the usual DOS, it is reasonable to adopt the WDOS function in most of the cases, since it yields relatively small (compared to CDOS) errors. In other words, the WDOS function gives a much more accurate representation for the true behavior of the DOS function than the CDOS for almost all ranges except the energies near to ground state energy. Hence, WDOS functions should be used in the calculation of physical properties of many systems ranging from nanometer–micro scale. This said, the DDOS may need to be used in the examination of high-confinement cases or systems having a large portion of particles near to the ground state, as near

**Figure 2.** Relative errors of WNOS for 10 different confinement values ranging from \( \alpha_1 = 0.1 \) to \( \alpha_1 = 1 \) varying with (a) energy (b) DNOS. For all cases other two directions are taken as nearly free so that \( \alpha_2 = \alpha_3 = 0.1 \).

**Figure 3.** Dimensionless internal energy changing with different confinement values. Black, dashed-cyan and orange curves represent internal energy values determined by discrete, Weyl and continuous DOS functions respectively. (a) Isometric confinement \( (\alpha_1 = \alpha_2 = \alpha_3 \text{ changes}) \), (b) 1D isometric \( (\alpha_1 = 0.05, \alpha_2 = \alpha_3 \text{ changes}) \), (c) 2D isometric \( (\alpha_1 = \alpha_2 = 0.05, \alpha_3 \text{ changes}) \), (d) anisometric \( (\alpha_1 = 0.05, \alpha_2 = 3, \alpha_3 \text{ changes}) \). Subfigures represent the relative error of internal energy calculated from WDOS for each particular case.
ground state properties can be more accurately predicted by using the DDOS function.

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