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Discrete density of states

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ABSTRACT

By considering the quantum-mechanically minimum allowable energy interval, we exactly count number of states (NOS) and introduce discrete density of states (DOS) concept for a particle in a box for various dimensions. Expressions for bounded and unbounded continua are analytically recovered from discrete ones. Even though substantial fluctuations prevail in discrete DOS, they're almost completely flattened out after summation or integration operation. It's seen that relative errors of analytical expressions of bounded/unbounded continua rapidly decrease for high NOS values (weak confinement or high energy conditions), while the proposed analytical expressions based on Weyl's conjecture always preserve their lower error characteristic.

1. Introduction

Density of states (DOS) is a useful concept that is extensively used in condensed matter and statistical physics. Although being a well-established and widely used concept, validity of conventional DOS is restricted by unbounded continuum approximation. Due to the rapid development of nanoscience and nanotechnology in recent years, detailed examination of DOS concept which is still commonly used in those areas became a necessity [1–7]. Moreover, advances in computational power of computers made it possible to exactly calculate the summations representing physical quantities, which is previously hard to do [7,8].

Essentially, state space is always discrete due to the finite size of domains and the wave character of particles. However, discreteness is usually neglected in case of the domain size is much larger than the de Broglie wavelength of particles, namely in macroscale. This leads to a continuous DOS (CDOS) function that is commonly used in literature. On the other hand, in nanoscale, at least one of the domain sizes is in the order of the de Broglie wavelength of particles and for such confined domains bounded continuum approximation represents the state space more properly. In a confined domain, bounded continuum approximation considers the non-zero value of ground states of momentum components while still neglecting their discrete nature. In this regard, Weyl's conjecture for the asymptotic behavior of eigenvalues uses bounded continuum approximation and offers a more precise enumeration of states; thus it gives a more accurate DOS function which may be called here Weyl DOS (WDOS).

Both CDOS and WDOS functions are based on continuum approximation, since they use infinitesimal energy interval assumption. However, quantum-mechanically minimum allowable energy interval is finite, and discrete nature of state space becomes significant when quantum confinement is strong. In this case, exact DOS function can only be defined by considering discrete energy eigenvalues. This treatment allows us to define discrete DOS (DDOS) function.

Long-standing unsolved "Gauss' circle problem" (or sphere in 3D case) that asks an analytical answer for "how many integer lattice points inside of a circle with a given radius" is profoundly related to the exact calculation of number of states in state space. Even though Gauss' circle and sphere problems are studied extensively for many years, still there are no exact analytical solutions in terms of elementary functions for both problems [9–11]. There are some studies related to these problems in literature for calculation of lattice sums [11–15]. Only a limited number of studies consider the evaluation of DOS functions for finite-size systems [5–7,9, 16–20]. On the other hand, they use approximations and assumptions instead of considering the exact energy interval to define DOS function. Also, none of them give an exact and discrete DOS function for a particle in a box which is one of the most fundamental models used in statistical physics.

The aim of this Letter is to introduce a discrete density of states function and to compare its results with conventional CDOS as well as Weyl's conjecture-based WDOS function that is proposed here. DDOS function is based on the exact enumeration of number of states (NOS) for quantum-mechanically allowable discrete energy

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levels, instead of using an infinitesimally small energy interval concept. In that sense, DDOS is the generalized form of DOS function which reduces to WDOS and CDOS functions in bounded and unbounded continuum limits respectively.

2. Generalized forms of DDOS, WDOS and CDOS functions for a particle in a box

As it is commonly preferred during the derivation of DOS in literature, we consider a non-interacting and non-relativistic massive particle confined in a D-dimensional rectangular domain. Dimensionless translational energy eigenvalues from the solution of Schrödinger equation for this kind of system are

$$\tilde{\varepsilon} = \frac{\varepsilon}{k_B T} = \frac{h^2}{8mk_B T}\sum_{n=1}^{D}\left(\frac{i_n}{L_n}\right)^2 = \sum_{n=1}^{D}(\alpha_n i_n)^2 \tag{1}$$

where D is the number of spatial dimensions, k_B is Boltzmann's constant, T is temperature, h is Planck's constant, m is single particle mass, n denotes orthogonal directions, L_n is length of the domain in nth direction and i_n is quantum state variable running from one to infinity. For convenience, we define here a confinement parameter α as $\alpha_n = h/\left(\sqrt{8mk_B T}L_n\right)$ to indicate the magnitude of confinement of the domain in direction n. It should be noted that, we use dimensionless energy throughout the derivations, $\tilde{\varepsilon} = \varepsilon/k_B T$, instead of energy itself for the simplicity of operations and the compactness of obtained expressions.

Let f be a Lebesgue-integrable function representing the physical quantity to be calculated. Summation of f over all accessible quantum states gives the physical quantity for the system. Apart from some exceptional cases, exact results of sums cannot be given analytically but only numerically. On the other hand, as long as confinement parameters are much smaller than unity, sums can be replaced by integrals with a negligible error, and thus analytical results can be obtained. Multiple sums turn into multiple integrals and CDOS function allows to calculate these multiple integrals over quantum state variables by a single integral over energy states,

$$\int_0^{\infty}\cdots\int_0^{\infty} f(\tilde{\varepsilon}_{i_1,\cdots i_D})di_1\cdots di_D = \int_0^{\infty} f(\tilde{\varepsilon})CDOS(\tilde{\varepsilon})d\tilde{\varepsilon} \tag{2}$$

where $CDOS(\tilde{\varepsilon}) = d\Omega_D/d\tilde{\varepsilon}$, $d\Omega_D$ is the number of states having energy values between $\tilde{\varepsilon}$ and $\tilde{\varepsilon}+d\tilde{\varepsilon}$ in D-dimensional space and $d\tilde{\varepsilon}$ is the infinitesimal energy interval.

On the contrary, when the confinement parameters are close to or even exceed unity, deviations between the results of integrals and sums become important. In this case, multiple summations may need to be exactly calculated instead of their integral approximations and DDOS function allows to calculate multiple summations by a single summation as long as energy eigenvalues are explicitly known. In that case, usage of DDOS function is given as follows

$$\sum_{i_1=1}^{\infty}\cdots\sum_{i_D=1}^{\infty} f(\tilde{\varepsilon}_{i_1,\cdots i_D})\Delta i_1\cdots\Delta i_D = \sum_{\tilde{\varepsilon}=\tilde{\varepsilon}_0}^{\infty} f(\tilde{\varepsilon})DDOS(\tilde{\varepsilon})\Delta\tilde{\varepsilon} \tag{3}$$

where $\tilde{\varepsilon}_0 = \alpha_1^2+\cdots+\alpha_D^2$ is ground state energy and $\Delta\tilde{\varepsilon}$ is the quantum-mechanically minimum allowable difference between successive energy levels, which is not a constant, unlike $d\tilde{\varepsilon}$. Unfortunately, it is not possible to obtain an analytical expression for $\Delta\tilde{\varepsilon}$ except for 1D case. Therefore, it is necessary to generate energy spectrum data by using Eq. (1) and apply ascending sorting process to this data, then calculate the exact energy intervals between successive energy levels numerically. Consequently, DDOS can be defined as,

$$DDOS_D(\tilde{\varepsilon}) = \frac{\Delta\Omega_D(\tilde{\varepsilon})}{\Delta\tilde{\varepsilon}} = \frac{\Omega_D(\tilde{\varepsilon}+\Delta\tilde{\varepsilon})-\Omega_D(\tilde{\varepsilon})}{\Delta\tilde{\varepsilon}} \tag{4}$$

where Ω_D is discrete number of states (DNOS) given by,

$$\Omega_D(\tilde{\varepsilon}) = DNOS_D(\tilde{\varepsilon}) = \sum_{i'_1=1}^{\infty}\cdots\sum_{i'_D=1}^{\infty}\Theta\left[\tilde{\varepsilon}-\sum_{n=1}^{D}(\alpha_n i'_n)^2\right] \tag{5}$$

where Θ is left-continuous Heaviside step function, $\Theta(0)=0$. It is clear that the difference of number of states for two successive energy levels ($\tilde{\varepsilon}$ and $\tilde{\varepsilon}+\Delta\tilde{\varepsilon}$) equal to the degeneracy of the energy level $\tilde{\varepsilon}$ since there are no states located in between successive energy levels. Note that, we consider spinless particles for brevity since spin degree of freedom is just a multiplication constant.

DDOS function predicts some exceptional results than those of CDOS function and it gives deeper physical insights which can be used in physical interpretations of non-trivial behaviors appeared in confined structures. While DDOS function gives an exact description for DOS function, it requires to know the shape of the domain and calculate the energy eigenvalues explicitly. In order to obtain an approximate DOS function for an arbitrary-shaped domain, the best approximation is to use Weyl's conjecture derived under bounded continuum approximation by neglecting discreteness. Weyl's conjecture that gives the asymptotic behavior of the number of eigenvalues less than k for Helmholtz wave equation (which is the stationary form of Schrödinger equation for a particle in a box) in a D-dimensional finite-size domain is commonly written as [3],

$$\Omega(k) = \frac{Vk^3}{6\pi^2}\Theta(D-2)+(-1)^D\frac{Sk^2}{4^{D-2}4\pi}\Theta(D-1) + (-1)^{D-1}\frac{Pk}{4^{D-1}\pi}\Theta(D)+(-1)^{D-2}\frac{N_E}{4^D} \tag{6}$$

where k is wavenumber, V, S, P and N_E are volume, surface, periphery and number of edges of the domain respectively. By considering parabolic dispersion relation between ε and k, we may obtain WNOS and WDOS functions respectively from Eq. (6) as,

$$WNOS_D(\tilde{\varepsilon}) = \sum_{\tilde{\varepsilon}_s}\left[\frac{4}{3\sqrt{\pi}}\frac{V}{\lambda_{th}^3}\tilde{\varepsilon}^{3/2}\Theta(D-2) + \frac{(-1)^D}{4^{D-2}}\frac{S}{\lambda_{th}^2}\tilde{\varepsilon}\Theta(D-1) + \frac{(-1)^{D-1}}{4^{D-1}}\frac{2}{\sqrt{\pi}}\frac{P}{\lambda_{th}}\sqrt{\tilde{\varepsilon}}\Theta(D)+\frac{(-1)^{D-2}}{4^D}N_E\right] \tag{7}$$

$$WDOS_D(\tilde{\varepsilon}) = \sum_{\tilde{\varepsilon}_s}\left[\frac{2}{\sqrt{\pi}}\frac{V}{\lambda_{th}^3}\sqrt{\tilde{\varepsilon}}\Theta(D-2)+\frac{(-1)^D}{4^{D-2}}\frac{S}{\lambda_{th}^2}\Theta(D-1) + \frac{(-1)^{D-1}}{4^{D-1}}\frac{1}{\sqrt{\pi}}\frac{P}{\lambda_{th}}\frac{1}{\sqrt{\tilde{\varepsilon}}}\Theta(D)\right] \tag{8}$$

where $\lambda_{th} = h/\sqrt{2\pi mk_B T}$ is thermal de Broglie wavelength, Heaviside step functions are left-continuous and $\tilde{\varepsilon}_s$ represents energy eigenvalues of subbands. Subbands are associated with quantized modes for confined directions of a domain. Hence, the number of confined directions denote the number of subband summations. *e.g.*, if the first direction is confined while the other two are free (quasi-2D), then $\tilde{\varepsilon}_s = (\alpha_1 i'_1)^2$ and there is one summation over i'_1; but if the first and second directions are confined and the other one is free (quasi-1D), then $\tilde{\varepsilon}_s = (\alpha_1 i'_1)^2+(\alpha_2 i'_2)^2$ and there is a double summation over i'_1 and i'_2.

CNOS and CDOS functions can be recovered from Eqs. (7) and (8) by neglecting higher order terms and considering rectangular domain geometry as follows,