Histogram Method for Density of States

Let the primitive unit cell be known and let it have volume V_c, then the Brillouin zone can be found and will have $V_b = (2\pi)^{\text{dim}}/V_c$ where dim is the dimension of the unit cell. Now, let the single-particle Hamiltonian be a matrix $H(k)$ with some finite size.

The histogram method to find the density of states is:

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initialize a histogram with bins for energy ranges
for point k in BZ discretization into N parts:
    diagonalize H(k); i.e. find its eigenvalues
    for eigenvalue E in eigenvalues:
        add 1 to the energy range E corresponds to
divide entire histogram by (N * V_c)
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where the result has units of $1/(\text{energy}\times\text{length}^{\text{dim}})$ in the relevant units.

This works because the density of states is:

$$D(E) = \int_{\text{BZ}} \frac{d^{\text{dim}}k}{(2\pi)^{\text{dim}}} \delta(E - E(k))$$

but $d^{\text{dim}}k \approx V_b/N = (2\pi)^{\text{dim}}/NV_c$, so:

$$D(E) \approx \sum_{n=1}^{N} \frac{\delta(E - E(k_n))}{NV_c}$$

which is precise in the limit of an infinite number of equally volumed elements $d^{\text{dim}}k$. Here, E corresponds to an energy bin, and $\delta(E - E(k_n)) = 1$ if $E(k_n)$ is in the energy bin and 0 otherwise.

More efficient methods exist, but the histogram method is simple to implement and is often fast enough to produce results reasonably quickly.