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Density of Surface States in Discrete Models

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We consider a simple quantum model with a surface and prove the existence of a surface density of states. We show that the energy spectrum of the model is the union of the support of the bulk densities of states of the media forming the surface and the support of the surface density of states.

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A simple but remarkably illuminating model of electron motion in a homogeneous medium is the discrete Schrödinger equation with wave functions defined on $\mathbb{Z}^n$ and with the Hamiltonian

$$(h_\omega u)(n) = \sum_{|j|=1} u(n+j) + V_\omega(n)u(n)$$
$$\equiv (h_0 u)(n) + V_\omega(n)u(n),$$

where the Hamiltonian h_ω and potential V_ω depend on a random parameter ω. Homogeneity is expressed by requiring V_ω to be an ergodic process. Examples include the Anderson model[1] [where the $V_0(n)$ are independent random variables] and periodic and almost periodic models.[2]

One of the basic quantities in this homogeneous case is the density-of-states measure, $dk(E)$, defined, for example, by

$$\int f(E)\,dk(E)$$
$$= \lim_{L\to\infty} (2L+1)^{-n} \sum_{|j_1|\le L,\ldots,|j_n|\le L} f(h_\omega)(j,j), \quad (1)$$

for smooth functions, f, of compact support [(j,j) refers to the diagonal matrix elements of the matrix $f(h_\omega)$]. The quantity dk is ω independent and the energy spectrum is given by

$$\mathrm{spec}(h_\omega) = \mathrm{supp}(dk).$$

These results are a simple consequence of the ergodic theorem proven, e.g., in Ref. 3.

In this Letter, we consider a model of a surface. Let $V_\omega^{(1)}(n)$, $V_{\omega'}^{(2)}(n)$ be two different bounded ergodic potentials[4] with associated bulk densities of states $dk^{(1)}$, $dk^{(2)}$. We will consider

$$\tilde h_{\omega,\omega'} = h_0 + V_{\omega,\omega'}(n),$$

where

$$V_{\omega,\omega'}(n) = \begin{cases} V_\omega^{(1)}(n), & n_1 \ge 0, \\ V_{\omega'}^{(2)}(n), & n_1 < 0, \end{cases}$$

so that $\tilde h$ describes a system with different media on each half-space with a surface in between. We will suppose that $n \ge 2$ and that $V_{\omega,\omega'}$ is ergodic under translations in $j_2, \ldots, j_n$.[5] Our main results are the following:

Theorem 1.—Under the above hypotheses, for any smooth f of compact support,

$$\lim_{L\to\infty} L^{-(n-1)} \left[\sum_{|j_k|\le L} f(\tilde h_{\omega,\omega'})(j,j) - (2L+1)^{n-1}(L+1)\int f(E)\,dk^{(1)}(E) - (2L+1)^{n-1}L\int f(E)\,dk^{(2)}(E) \right] \quad (2)$$

exists, is independent of ω,ω', and defines a distribution $T(f)$.

This theorem says that if you compare the set of states for the system with a surface and the half-space bulk density, the difference is a surface term, and thus defines a natural surface density of states.

Theorem 2.—

$$\mathrm{spec}(\tilde{h}_{\omega,\omega'}) = \mathrm{supp}(dk_1) \cup \mathrm{supp}(dk_2) \cup \mathrm{supp}(T).$$

This theorem says that the allowed energies can be associated with either the bulk medium or the surface.

Unlike $dk^{(j)}$, T is certainly not a positive measure, since its average $T(1)$ is zero. It might be a signed measure, but we do not have a proof of such a fact.[6] That is, we know that T is finite when averaged with a smooth function, f, but we do not know how to prove that it has a finite density. While one can prove that T is nonzero in some explicit cases with periodic potentials, we do not have a general proof that it is nonvanishing. Detailed proofs of these results, and discussion of the continuum case, will appear elsewhere.[7]

Here is a sketch of the proof.[8]

Step 1: Let $P_t(j) = e^{it\tilde{h}}(j,j)$, the propagator for $\tilde{h}$, and $P_t^{(i)}(j)$, $i=1,2$, the same for $V^{(1)},V^{(2)}$ defined globally. Let

$$\Delta P_t(j) = \begin{cases} P_t(j) - P_t^{(1)}(j), & j_1 \geq 0, \\ P_t(j) - P_t^{(2)}(j), & j_1 < 0. \end{cases}$$

We expand $e^{it(h_0+V)}$ in a perturbation series about e^{itV}. Since h_0 only couples nearest neighbors, only perturbation terms of order $n \geq |j_1|$ enter. Thus

$$|\Delta P_t(j)| \leq 2 \sum_{|n| \geq j_1} (n!)^{-1}(2dt)^n,$$

so that, for $j_1 \geq 32(dt)^2$, one sees that

$$|\Delta P_t(j)| \leq 4(\tfrac{1}{2})^{|j_1|}.$$

For any j,

$$|\Delta P_t(j)| \leq 2.$$

Step 2: With use of this estimate,

$$\sum_{j_1} |\Delta P_t(j)| \leq 128(dt)^2 + 8.$$

Step 3: Note that the quantity (2) can be written in terms of $\hat{f}$, the Fourier transform of f, by

$$L^{-(n-1)} \sum_{|j_k| \leq L} (2\pi)^{-1/2} \int \hat{f}(s) \Delta P_s(j)\, ds,$$

so that, if $\int |\hat{f}(s)| s^2 ds < \infty$ (certainly true if f is infinitely smooth), the existence of the limit follows from the ergodic theorem.

Step 4: Given the arguments above, theorem 2 follows, as in the bulk case.[3]

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[1] H. Kunz and B. Souillard, Commun. Math. Phys. **78**, 201 (1980).

[2] J. Avron and B. Simon, Duke Math. J. **50**, 369 (1983).

[3] L. Pastur, Commun. Math. Phys. **75**, 179 (1980), and Usp. Mat. Nauk. **28**, 3 (1973).

[4] For example, one can take $V^{(1)}=0$, corresponding to a half-space filled with medium 2.

[5] This is true, for example, if both $V^{(1)}$ and $V^{(2)}$ are Anderson models (including one of them identically zero). But, for example, it is false if $V^{(1)}$ and $V^{(2)}$ are periodic, and H. Englisch, W. Kirsch, M. Schroder, and B. Simon, to be published, will discuss the case where less is known.

[6] In the one case that we can compute [$V^{(1)},V^{(2)}$ periodic; see, e.g., E. B. Davies and B. Simon, Commun. Math. Phys. **63**, 277 (1978)], T is a signed measure, and has the form $f(E)dE$.

[7] Englisch *et al.*, Ref. 5.

[8] Englisch *et al.* (Ref. 5) will also discuss the continuum case, where the simple perturbation series in h_0 cannot work since h_0 is singular relative to e^{isV}. We instead need to combine path-integral methods with some subtle functional analysis.