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Asymptotic Series for the Ground State Energy of Schrödinger Operators*

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We find sufficient conditions for the ground state energy $e(\lambda)$ of $-\Delta+\lambda V$ to have an asymptotic series $\sum a_n\lambda^n$ as $\lambda\downarrow 0$. Included are a class of almost periodic functions.

1. INTRODUCTION

We study here the ground state energy $e(\lambda)$ of a Schrödinger operator $-\Delta+\lambda V$ about $\lambda=0$, a subject we've also looked at in [1]. Here we will look at conditions that yield an asymptotic series. The problem is subtle because $-\Delta$ has zero at the bottom of its essential spectrum and the usual projection methods [3] for obtaining asymptotic series fail. In essence our main result assumes one can solve for formal Rayleigh–Schrödinger ground states.

THEOREM 1. *Suppose there exist $C^2(\mathbb{R}^\nu)$ functions uniformly bounded, $Z_1, ..., Z_N$ and constant $c_1, ..., c_N$, so that* $(Z_0\equiv 1)$, for $n=1, ..., N$

$$\Delta Z_n = VZ_{n-1}-\sum_{i=1}^{n} c_i Z_{n-i}. \tag{1}$$

Then $e(\lambda)=\sum_{j=1}^{N} c_j\lambda^j+O(\lambda^{N+1})$.

This theorem is applicable to certain almost periodic functions so we'll prove some results for that case. As a preliminary to stating our result, we need to define a notion of good Diophantine matrices. Let $A\colon\mathbb{R}^\nu\to\mathbb{R}^\mu$ be a linear transformation. Let $\mathscr{L}\subset\mathbb{R}^\mu$ be a full lattice, i.e., a discrete subgroup, so $\mathbb{R}^\mu/\mathscr{L}$ is compact ($\mathscr{L}$ is μ-dimensional). We say that A has

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good Diophantine properties mod $\mathscr{L}$ if and only if there exist C, $\alpha > 0$ so that

$$\|A^t l\| \geqslant C\,|l|^{-\alpha} \tag{2}$$

for all $l \in \mathscr{L}\backslash\{0\}$. Given a lattice $\mathscr{L}$ in $\mathbb{R}^\mu$, we define as usual the dual $\mathscr{L}^*$ by $\beta \in \mathscr{L}^*$ if and only if $\langle \beta, \alpha \rangle \in \mathbb{Z}$ for all $\alpha \in \mathscr{L}$.

THEOREM 2. *Suppose that either V is a finite trigonometric polynomial $V(\mathbf{x}) = \sum_{n=-N}^{N} a_n e^{i\boldsymbol{\alpha}_n \cdot \mathbf{x}}$; $\boldsymbol{\alpha}_n$ arbitrary with $\boldsymbol{\alpha}_{-n} = -\boldsymbol{\alpha}_n$; $a_{-n} = \bar{a}_n$, or*

$$V(x) = f(Ax)$$

with $f \in C^\infty$ and $\mathscr{L}$-periodic on $\mathbb{R}^\mu$ and that A has good Diophantine properties mod $\mathscr{L}^*$. *Then $e(\lambda)$, the ground state of $-\Delta + \lambda V$, has an asymptotic series about* 0 *to all orders.*

In Section 2, we present a simple theorem to show that a suitable approximate ground state implies an error estimate on the energy. In Section 3, we use this to prove Theorem 1; and in Section 4 we prove Theorem 2. For results related to Theorem 2, see Kozlov [2].

2. Approximate Ground States and Approximate Energies

We will prove Theorem 1 by constructing an approximate ground state. We'll need the following result to go from the appproximate eigenvector to an approximate energy.

THEOREM 3. *Let V be a bounded potential on $\mathbb{R}^\nu$. Suppose there exists a positive polynomially bounded function u on $\mathbb{R}^\nu$, a real number E, and function $g \in L^\infty$, so that*

$$(-\Delta + V - E)\,u = gu.$$

Then

$$|e(V) - E| \leqslant \|g\|_\infty.$$

Proof. Let $W = V - g$. Then u is an eigenfunction of $-\Delta + W$ with eigenvalue E. Since u is polynomially bounded, Schnol's theorem (see, e.g., [4]) implies $E \in \sigma(-\Delta + W)$. Since $u > 0$, the Allegretto–Piepenbrink theorem (see, e.g., [4]) implies $-\Delta + W \geqslant E$. It follows that $E = \inf \sigma(-\Delta + W)$. Since $\|(-\Delta + V) - (-\Delta + W)\| \leqslant \|g\|_\infty$, the proof is complete. ∎

3. Proof of Theorem 1

Let $u = \sum_{n=0}^{N} \lambda^n Z_n$. Then, by (1)

$$\Delta u = \sum_{n=1}^{N} \lambda^n V Z_{n-1} - \sum_{n=1}^{N} \sum_{i=1}^{n} c_i \lambda^i \lambda^{n-i} Z_{n-i}$$

$$= (\lambda V) u - \lambda^{N+1} V Z_N - \left(\sum_{i=1}^{N} c_i \lambda^i \right) \left(\sum_{j=0}^{N} \lambda^j Z_j \right)$$

$$+ \sum_{\substack{1 \leqslant i \leqslant N \\ 0 \leqslant j \leqslant N \\ i+j > N}} c_i Z_j \lambda^{i+j}.$$

Thus

$$\left[-\Delta + \lambda V - \left(\sum_{i=1}^{N} c_i \lambda_i \right) \right] u = G,$$

where $G = O(\lambda^{N+1})$. Since $u = 1 + O(\lambda)$ for λ small, u^{-1} is uniformly bounded so $g = G u^{-1}$ is $O(\lambda^{N+1})$. Now use Theorem 3. ▮

4. Proof of Theorem 2

Consider first the case where V is a finite trigonometric polynomial. We want to solve Eq. (1) inductively, that is, given $Z_1, \ldots, Z_{n-1}$ and $c_1, \ldots, c_{n-1}$ find Z_n and c_n. As part of the induction, we suppose also that $Z_1, \ldots, Z_{n-1}$ are finite trigonometric polynomials. By this induction hypothesis,

$$V Z_{n-1} - \sum_{i=1}^{n-1} c_i Z_{n-i} \equiv W_n$$

is a finite trigonometric polynomial, say

$$W_n(x) = \sum_{j=-N_n}^{N_n} a_j e^{i\alpha_j \cdot x}$$

with $\alpha_0 = 0$. Just take

$$c_n = a_0; \qquad Z_n = -\sum_{j \neq 0} a_j \, |\alpha_j|^{-2} \, e^{i\alpha_j \cdot x}.$$

This completes the induction and so the proof of Theorem 1 in this case.

So we turn to the case of smooth quasiperiodic functions with good

Diophantine properties. Given a function g on $\mathbb{R}^\mu/\mathscr{L}$, we can make a Fourier expansion

$$g(y) = \sum_{k \in 2\pi\mathscr{L}^*} a_k e^{ik \cdot y}.$$

We define $M\colon L^\infty(\mathbb{R}^\mu/\mathscr{L}) \to L^\infty(\mathbb{R}^\nu)$ by $(Mg)(x) = g(Ax)$. We define $\mathscr{D}$ on smooth functions on $\mathbb{R}^\mu/\mathscr{L}$ by

$$(\mathscr{D}g)(y) = -\sum_k a_k \, \|A^t k\|^2 \, e^{ik \cdot y}$$

so that

$$\Delta(Mg) = M(\mathscr{D}g).$$

Suppose we find C^∞ functions $g_1, ..., g_n$ on $\mathbb{R}^\mu/\mathscr{L}$ and $c_1, ..., c_n$ so that (with $g_0 \equiv 1$)

$$\mathscr{D}g_n = fg_{n-1} - \sum_{i=1}^{n} c_i g_{n-i}.$$

Then $Z_n = Mg_n$ obeys (1) and the theorem is proven. By induction we suppose $g_1, ..., g_{n-1}$ are C^∞. Then

$$W_n = fg_{n-1} - \sum_{i=1}^{n-1} c_i g_{n-i}$$

is C^∞. Let

$$W_n = \sum_{k \in 2\pi\mathscr{L}^*} a_k^{(n)} e^{iky}.$$

Then we take

$$c_n = a_0^{(n)}$$

$$g_n = \sum_{k \neq 0} \|A^t k\|^{-2} \, a_k^{(n)} e^{iky}.$$

By the Diophantine hypothesis (2)

$$\|A^t k\|^{-2} \leqslant C\,|k|^{2\alpha}.$$

Since W_n is C^∞,

$$|a_k^{(n)}| \leqslant D_{n,l}\,|k|^{-l}$$

for all $l > 0$. So

$$\|A'k\|^{-2} |a_k^{(n)}| \leqslant D_{n,l} |k|^{-l+2\alpha}$$

and thus g_n is C^∞. ∎

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