SCHRÖDINGER OPERATORS IN THE TWENTY-FIRST CENTURY

BARRY SIMON

1. Introduction

Yogi Berra is reputed to have said, "Prediction is difficult, especially about the future." Lists of open problems are typically lists of problems on which you expect progress in a reasonable time scale and so they involve an element of prediction.

We have seen remarkable progress in the past fifty years in our understanding of Schrödinger operators, as I discussed in Simon [1]. In this companion piece, I present fifteen open problems. In 1984, I presented a list of open problem in Mathematical Physics, including thirteen in Schrödinger operators. Depending on how you count (since some are multiple), five have been solved.

We will focus on two main areas: anomalous transport (Section 2) where I expect progress in my lifetime, and Coulomb energies where some of the problems are so vast and so far from current technology that I do not expect them to be solved in my lifetime. (There is a story behind the use of this phrase. I have heard that when Jeans lectured in Göttingen around 1910 on his conjecture on the number of nodes in a cavity, Hilbert remarked that it was an interesting problem but it would not be solved in his lifetime. Two years later, Hilbert's own student, Weyl, solved the problem using in part techniques pioneered by Hilbert. So I figure the use of that phrase is a good jinx!)

In a final section, I present two other problems.

2. Quantum Transport and Anomalous Spectral Behavior

For the past twenty-five years, a major thrust has involved the study of Schrödinger operators with ergodic potentials and unexpected spectral behavior of Schrödinger operators in slowly decaying potentials. (This is discussed in Sections 5 and 7 of Simon [1].) The simplest models of ergodic Schrödinger operators involve finite difference approximations. The first is the prototypical random model and the second, the prototypical almost periodic model.

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Example 2.1. (Anderson model) *Let $V_\omega(n)$ be a multisequence of independent, identically distributed random variables with distribution uniform on $[a,b]$. Here $n \in \mathbb{Z}^\nu$ is the multisequence label and ω the stochastic label. On $\ell^2(\mathbb{Z}^\nu)$, define*

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

Example 2.2. (Almost Mathieu equation) *On $\ell^2(\mathbb{Z})$, define*

$$(h_{\alpha,\lambda,\theta}u)(n) = u(n+1) + u(n-1) + \lambda\cos(\pi\alpha n + \theta)u(n).$$

Here α, λ are fixed parameters where α is usually required to be irrational and λ is a coupling constant. θ runs in $[0, 2\pi)$ and plays a role similar to the ω of Example 2.1.

It is known that the Anderson model has spectrum $[a-2\nu, b+2\nu]$ and that if $\nu = 1$, the spectrum is dense pure point with probability 1, and if $\nu \geq 2$, this is true if $|b-a|$ is large enough (we will not try to recount the history here; see Simon [2] for proofs of these facts and some history) and also there is some pure point spectrum near the edges of the spectrum when $|b-a|$ is small.

Problem 1. (Extended states) Prove for $\nu \geq 3$ and suitable values of $b-a$ that the Anderson model has purely absolutely continuous spectrum in some energy range.

This is the big kahuna of this area, the problem whose solution will make a splash outside the field. In fact, just proving that there is any a.c. spectrum will cause a big stir. The belief is that for $|b-a|$ small, there is a subinterval $(c,d) \subset [a-2\nu, b+2\nu] = \sigma(H_\omega)$ on which the spectum is purely a.c. and that on the complement of this interval, the spectrum is dense pure point. As $|b-a|$ increases beyond a critical value, $|d-c|$ goes to zero.

Problem 2. (Localization in two dimensions) Prove that for $\nu = 2$, the spectrum of the Anderson model is dense pure point for all values of $b-a$.

This is the general belief among physicists, although the claims for this model have fluctuated in time.

Problem 3. (Quantum diffusion) Prove that for $\nu \geq 3$ and values of $|b-a|$ where there is a.c. spectrum that $\sum_{n\in\mathbb{Z}^\nu} n^2 |e^{itH}(n,0)|^2$ grows as $c\,t$ as $t \to \infty$.

That is, $\langle x(t)^2\rangle^{1/2} \sim \tilde{c}\,t^{1/2}$. For scattering states, of course, the a.c. spectrum leads to ballistic behavior (i.e., $\langle x(t)^2\rangle^{1/2} \sim c\,t$) rather than diffusive behavior. This problem is one of a large number of issues concerning the long time dynamics of Schrödinger operators with unusual spectral properties.

An enormous amount is now known about the almost Mathieu model whose study is a fascinating laboratory. I would mention three remaining problems about it:

Problem 4. (Ten Martini problem) Prove for all $\lambda \neq 0$ and all irrational α that $\mathrm{spec}(h_{\alpha,\lambda,\theta})$ (which is θ independent) is a Cantor set, that is, that it is nowhere dense.

The problem name comes from an offer of Mark Kac. Bellissard-Simon [3] proved the weak form of this for Baire generic pairs of (α, λ). It would be interesting to prove this even just at the self-dual point $\lambda = 2$.

Problem 5. Prove for all irrational α and $\lambda = 2$ that $\mathrm{spec}(h_{\alpha,\lambda,\theta})$ has measure zero.

This is known (Last [4]) for all irrational α's whose continued fraction expansion has unbounded entries. But it is open for α the golden mean which is the value with the most numerical evidence! To prove this, one will need a new understanding of the problem.

Problem 6. Prove for all irrational α and $\lambda < 2$ that the spectrum is purely absolutely continuous.

It is known (Last [5], Gesztesy-Simon [6]) that the Lebesgue measure of the a.c. spectrum is the same as the typical Lebesgue measure of the spectrum for all irrational α and $\lambda < 2$. The result is known (Jitomirskaya [7]) for all α's with good Diophantine properties but is open for other α's. One will need a new understanding of a.c. spectrum to handle the case of Louiville α's.

While we have focused on the almost Mathieu equation, the general almost periodic problem needs more understanding. As for slowly decaying potentials, I will mention two problems:

Problem 7. Do there exist potentials $V(x)$ on $[0, \infty)$ so that $|V(x)| \leq C|x|^{-1/2-\varepsilon}$ for some $\varepsilon > 0$ and so that $-\frac{d^2}{dx^2} + V$ has some singular continuous spectrum.

It is known that such models always have a.c. spectrum on all of $[0, \infty)$ (Remling [8], Christ-Kiselev [9], Deift-Killip [10], Killip [11]). It is also known (Naboko [12], Simon [13]) that such models can also have dense point spectrum. Can they have singular continuous spectrum as well?

Problem 8. Let V be a function on $\mathbb{R}^\nu$ which obeys

$$\int |x|^{-\nu+1} |V(x)|^2 \, d^\nu x < \infty.$$

Prove that $-\Delta + V$ has a.c. spectrum of infinite multiplicity on $[0, \infty)$ if $\nu \geq 2$.

If $\nu = 1$, this is the result of Deift-Killip [10] (see also Killip [11]). Their result implies the conjecture in this problem for spherically symmetric potentials (which is where the $|x|^{-\nu+1}$ comes from).

3. Coulomb Energies

The past thirty-five years have seen impressive development in the study of energies of Schrödinger operators with Coulomb potentials (see Sections 9 and 11 of Simon [1] or the review of Lieb [14]) of which the high points were stability of matter, the three-term asymptotics of the total binding energy of a large atom, and some considerable information on how many electrons a given nucleus can bind.

While these results involve deep mathematics, except for stability of matter, they are very remote from problems of real physics. Since one does not often fully ionize an atom, total binding energies are not important, but rather single ionization energies are. Understanding the binding energies of atoms and molecules is a huge task for mathematical physics. The problems in this section may be signposts along the way. As we progress, the problems will get less specific. We will deal throughout with fermion electrons. $\mathcal{H}_f^{(N)}$ will be the space of functions antisymmetric in spin and space in $L^2(\mathbb{R}^{3N};\mathbb{C}^{2N})$.

Define $H(N,Z)$ to be the Hamiltonian on $\mathcal{H}_f$,

$$\sum_{i=1}^{N}\left(-\Delta_i - \frac{Z}{|x_i|}\right) + \sum_{i<j}\frac{1}{|x_i - x_j|}$$

and

$$E(N,Z) = \min_{\mathcal{H}_f} H(N,Z).$$

$N_0(Z)$ is defined to be the smallest value of N for which $E(N+j,Z) = E(N,Z)$ for $j = 1,2,3,\dots$. Ruskai [15, 16] and Sigal [17, 18] showed such an $N_0(Z)$ exists. Lieb [19] showed that $N_0(Z) \le 2Z$ and Lieb *et al.* [20] that $N(Z)/Z \to 1$ as Z goes to infinity. By Zhislin [21], we know $N_0(Z) \ge Z$.

Problem 9. Prove that $N_0(Z) - Z$ is bounded as $Z \to \infty$.

It is not an unreasonable conjecture that $N_0(Z)$ is always either Z or $Z+1$.

One has (see Simon [1] for detailed references)

$$E(Z) \equiv \min_N E(N,z) = aZ^{7/3} + bZ^2 + cZ^{5/3} + o(Z^{5/3}),$$

but more physically significant is the ionization energy

$$(\delta E)(Z) = E(Z, Z-1) - E(Z,Z).$$

Problem 10. What is the asymptotics of $(\delta E)(Z)$ as $Z \to \infty$?

There is a closely related issue: to define a radius of an atom (perhaps that $R(Z)$ so that $N-1$ electrons are within the ball of radius R) and determine the asymptotics of $R(Z)$.

Problem 11. Make mathematical sense of the shell model of an atom.

This is a vague problem, but the issue is what does the most popular model used by atomic physicists and chemical physicists have to do with the exact quantum theory.

Here is an even vaguer problem:

Problem 12. Is there a mathematical sense in which one can justify from first principles current techniques for determining molecular configurations?

Drug designers and others use computer programs that claim to determine configurations of fairly large molecules. While one technique these programs use is called *ab initio*, all that means is they use few parameter molecular orbitals. This problem should be viewed as asking for some precise way to go from fundamental quantum theory to configuration of macromolecules.

Finally,

Problem 13. Prove that the ground state of some neutral system of molecules and electrons approaches a periodic limit as the number of nuclei goes to infinity.

That is, prove crystals exist from first quantum principles.

4. Other Problems

Here are two final open problems:

Problem 14. Prove the integrated density of states, $k(E)$, is continuous in the energy.

For a definition of $k(E)$, see Cycon *et al.* [22]. Continuity is known in one dimension and for the discrete case, but has been open in the higher-dimensional continuum case for over fifteen years.

Problem 15. Prove the Lieb-Thirring conjecture on their constants $L_{\gamma,\nu}$ for $\nu = 1$ and $\frac{1}{2} < \gamma < \frac{3}{2}$.

$L_{\gamma,\nu}$ is defined to be the smallest constant so that

$$\sum_j |e_j(V)|^\gamma \leq L_{\gamma,\nu} \int dx |V(x)|^{\gamma+\nu/2}\, d^\nu x,$$

where $e_j(V)$ is the jth negative eigenvalues of $-\Delta + V$ on $L^2(\mathbb{R}^\nu)$.

Here $\gamma \geq \frac{1}{2}$ in $\nu = 1$ dimension and $\gamma \geq 0$ in dimensions ≥ 2. Two lower bounds on $L_{\gamma,\nu}$ can be computed—the quasiclassical value $L^{\text{q.c.}}_{\gamma,\nu}$ and the best constant, $L^{\text{Sob}}_{\gamma,\nu}$ for one bound state (which is related to best constants in Sobolev inequalities). For $\nu = 1$, Lieb-Thirring [23] conjectured

$$L_{\gamma,\nu} = \max(L^{\text{q.c.}}_{\gamma,\nu}, L^{\text{Sob}}_{\gamma,\nu})$$

which is $L^{\text{q.c.}}_{\gamma,\nu}$ if $\gamma \geq \frac{3}{2}$ and $L^{\text{Sob}}_{\gamma,\nu}$ if $\frac{1}{2} \leq \nu \leq \frac{3}{2}$. The conjecture is known to hold if $\gamma \geq \frac{3}{2}$ (Aizenman-Lieb [24]) and if $\gamma = \frac{1}{2}$ (Hundertmark-Lieb-Thomas [25]). Also open is the best value of the constant if $\nu \geq 2$ and $0 \leq \gamma < \frac{3}{2}$. It is known that if $\nu \geq 8$ and $\gamma = 0$, $L_{\gamma,\nu} > \max(L^{\text{q.c.}}_{\gamma,\nu}, L^{\text{Sob}}_{\gamma,\nu})$ with strict inequality.

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Division of Physics, Mathematics, and Astronomy, 253-37, California Institute of Technology, Pasadena, CA 91125, USA, E-mail: bsimon@caltech.edu