QFT METHODS FOR STUDYING THE DENSITY OF RESONANCES IN OPEN DISORDERED MULTIDIMENSIONAL SYSTEMS Joshua Feinberg

University of Haifa at Oranim and Technion

PHHQPXII, 24 June 2011, Max Planck Inst., Dresden

OUTLINE

- Introduction: resonances and their relevance to studying disordered systems.
- The effective nonhermitian hamiltonian, outgoing waves.
- Averaging over disorder the SUSY Method (hermitian case)
- Averaging over non-hermitian operators the Method of Hermitization.
- The SUSY method applied to the hermitized disordered effective hamiltonian.

A CLOSED DISORDERED SYSTEM

closed system: real energy eigenvalues E_{α} eigenstates ψ_{α} $H\psi_{\alpha}=E_{\alpha}\psi_{\alpha}$

 $\psi_{\alpha}(x)$ either localized (typically exponentially) with localization length (inverse Lyapunov exponent) $\xi(E_{\alpha})$, or extended throughout the system

In Id & 2d localized for all energies (albeit in 2d localization length can be extremely huge, bigger than the size of any conceivable system). In 3d there is a genuine transition (the Anderson transition) between localized states (between the band and mobility edges) and extended states (in the middle of the energy band).

CONNECT THE SYSTEM TO THE OUTER WORLD:

A particle, initially trapped in the system, may escape out through the lead. This phenomenon corresponds to a quasi-stationary state - a resonance.

- The original eigenstate ψ_{α} of the closed system, with energy E_{α} , has become a resonance, with complex energy $z_{\alpha} = \tilde{E}_{\alpha} - \frac{i}{2}\Gamma_{\alpha}$
- The stronger the original state $\psi_{\alpha}(\mathbf{r})$ "feels" the opening of the system (say, at $\mathbf{r} = 0$), the greater probability of the particle to escape.
- Thus, expect eigenstates, whose amplitudes near the opening, $|\psi_{\alpha}(0)|$, are large, to develop large resonance widths Γ_{α} , and vice versa.

- strongly localized states in the original system => narrow resonances
- extended states => large resonance widths
- Γ is reminiscent of Thouless' criterion for localization (in closed systems) check sensitivity to the boundary conditions: change b.c. slightly, then $E_{\alpha} \rightarrow E_{\alpha} + \delta E_{\alpha}$. Let $\Delta =$ mean level spacing. Then, if we have $\left|\frac{\delta E_{\alpha}}{\Delta}\right| \ll 1$, the state is localized.
- sensitivity of the imaginary part of the complex energy eigenvalue to b.c. and its consequent interpretation are reminiscent of a similar phenomenon in the Hatano-Nelson model.

could this analogy with standard localization theory pushed further? $\Delta \sim L^{-d} E^{1-\frac{d}{2}}$ where L is the system's size, and d is dimensionality

conjecture:

I.Strong disorder (strongly localized states): $\Gamma \sim |\psi(0)|^2 \sim e^{-\frac{L}{\xi}}$ thus $\frac{\Gamma}{\Lambda} \sim L^d e^{-\frac{L}{\xi(E)}} E^{\frac{d}{2}-1}$

2. Diffusive regime: $\Gamma \sim \frac{D}{L^2}$, D diffusion coefficient $\frac{\Gamma}{\Lambda} \sim (L\sqrt{E})^{d-2} \cdot D$ 3. Scaling regime (near the Anderson transition): $\Gamma \sim D \sim L^{-d}$

 $\frac{\Gamma}{D}$ scale invariant

In order to answer all these questions, we need to compute the averaged density of resonances (DOR):

$$o(E,\Gamma) = \langle \sum_{\alpha} \delta(E - E_{\alpha}) \delta(\Gamma - \Gamma_{\alpha}) \rangle$$

$$z = E - \frac{i}{2}\Gamma$$
 is the complex energy

This is a one-point correlator (as opposed to the 2-point function $\langle G_{ret}G_{adv}\rangle$ typically studied in the hermitian case). Again, a situation very similar to what one studies in the Hatano-Nelson model.

The Effective Hamiltonian

Resonance complex energies could be thought of as the complex eigenvalues of a nonhermitian effective hamiltonian H_{eff} . The outer world is eliminated and one reformulates the problem entirely in terms of the degrees of freedom of the original system and its coupling to the outer world. The DOR is thus the density of eigenvalues of this nonhermitian hamiltonian.

Description of open quantum systems in terms of effective nonhermitian hamiltonians has a long history:
 Feshbach; Wiedenmueller, Zirnbauer & Verbaarschot, Rotter et al., Fyodorov and Sommers, Datta and more. These (save for Datta's book) are largely based on manipulating the S-matrix of the system, depending on how many scattering channles are opened and connect the system to the outer world. This, of course depends on energy. Hence, H_{eff} is inevitably energy dependent.

Let us now derive the effective nonhermitian hamiltonian:

RESONANCES AS STATIONARY OUTGOING WAVE SOLUTIONS OF THE SCHRODINGER EQUATION

- Work in the continuum directly.
- Solve the Schrodinger Equation $H\psi = E\psi$ inside the system, subjected to the boundary condition that the wave outside the system be a freely propagating outgoing wave.
- This determines the value of the wave function right outside the system's boundary. Once this is done we can forget about the environment, cut it out, and restrict the Hamiltonian to the domain of the system.
- We shall further assume a tunneling barrier at the system's boundary.



- This boundary condition clearly renders the Hamiltonian nonhermitian: the particle tunnels out of the system.
- This is known also as Sievert's boundary condition.
- This is how Gamow originally explained nuclear alpha decay.
- It is completely equivalent to the description of resonances as poles of the S-matrix in the un-physical sheet.

EXAMPLE: THE EFFECTIVE RESONANCE HAMILTONIAN IN 1D IN THE CONTINUUM

The disordered system lives in the segment [0,L]. The right end at x=L is closed (Dirichlet boundary condition). The particle can tunnel out of the system through a tunneling barrier located at x=0, and escape into a perfect lead stretching along the negative axis, in which it propagates freely to the left.

The hamiltonian inside the system is

$$H_{system} = \frac{p^2}{2m} + V(x) + g\delta(x), \quad 0 \le x \le L, g > 0$$

The last term is the tunneling barrier. We impose Dirichlet b.c. at the closed end: $\,\psi(L)=0$

Free propagation to the left in the lead: $\psi(x) = \psi(0) e^{-ikx}$, $E = \frac{\hbar^2 k^2}{2m}$, $\operatorname{Re} k > 0$

12

Thus, just outside the system, into the lead, $\ \psi'(0-)=-ik\psi(0)$

The derivative has to jump across the tunneling barrier. One finds a Robin-type complex and **energy dependent** boundary condition:

$$\psi'(0+) + (ik+\lambda)\psi(0) = 0, \quad \lambda = -\frac{2mg}{\hbar^2} < 0$$

Monday, July 11, 2011

Clearly, we can now eliminate the lead altogether, and solve the Schrodinger Equation

 $\left(\frac{p^2}{2m} + V(x)\right)\psi(x) = \frac{\hbar^2k^2}{2m}\psi(x) \quad \text{ only inside the system 0<x<L,}$

subjected to the boundary condition $\psi'(0+) + (ik + \lambda)\psi(0) = 0$ where of course, $\operatorname{Re} k > 0$ and $\lambda < 0$

(and to the Dirichlet b.c. at the other end).

The Schrodinger operator together with the complex energy-dependent boundary condition define the nonhermitian effective hamiltonian H_{eff} for resonances in this simple system.

As an easy exercise, to see what's going on, just work out the case V=0

LET US MAKE A FEW COMMENTS:

- The LHS of the boundary condition $\psi'(0+) + (ik + \lambda)\psi(0)$ is really the spectral determinant of the problem:
- It depends on the energy through k.
- Integrate the Schrodinger equation with initial conditions $\psi(L) = 0$, $\psi'(L) = 1$ to the left, into the system. Call the solution $\psi(x; k)$.
- Then impose the boundary condition at x=0, which is the spectral condition on k.

THIS 1D MODEL CAN BE EASILY GENERALIZED TO HIGHER DIMENSIONS:

For example, consider a 3d infinite slab of disordered material, located between 0<z<L. The system is closed at the plane z=L, and is connected to the outside world through a tunneling barrier, which is the entire plane z=0. The outside world is a perfect conductor, where the particle propagates freely.



Obtain the boundary condition

 $\left[\partial_z \psi + (\lambda + iq \operatorname{sign} \operatorname{Im}(q))\psi\right]_{|z=0+} = 0$

where

$$q^2 = \frac{2m\zeta}{\hbar^2} - \mathbf{k}_\perp^2$$

The Schrodinger hamiltonian inside the slab 0<z<L, together with the resonance b.c. at z=0 (and the Dirichlet b.c. at z=L) comprise the desired effective hamiltonian for this system.

Note that the resonance b.c. is independent of the direction $\hat{\mathbf{k}}_{\perp}$, reflecting rotational symmetry (of the outside world) about the *z*-axis.

As another example, consider disordered system in the shape of a sphere of radius R, centered at the origin. The sphere's surface is a tunneling barrier. An electron initially in the disordered ball can tunnel through the barrier, and escape to freedom.

Due to spherical symmetry, resonances may be decomposed into definite angular momentum states ψ_{lm} . Let us consider such a resonance with complex energy $\zeta = \frac{\hbar^2 Q^2}{2m}$. The resonance b.c. at the sphere at r=R is



17

HOW TO OBTAIN THE RESONANCE B.C. IN GENERAL?

It is possible to derive a master formula (M. Zirnbauer) Let $\partial \Omega$ be the system's boundary, coordinated by ξ

 $G^{(+)}\left({f r},{f r}';\zeta
ight)$

the exact Green's function of the system, with outgoing wave b.c., at complex energy

 $G_{D}^{(+)}\left({f r},{f r}^{\prime};\zeta
ight)$

the exact outgoing wave Green's function of the system, with **Dirichlet** b.c. at $\partial \Omega$

observation point



environment



MASTER FORMULA:

 $G^{(+)}(\mathbf{r},\mathbf{r}';\zeta) = -\frac{\hbar^2}{2m} \int_{\partial\Omega} d^2\xi \left(\hat{n}_{\xi} \cdot \nabla_{\xi} G_D^{(+)}(\xi,\mathbf{r};\zeta) \right) G^{(+)}(\xi,\mathbf{r}';\zeta)$ \uparrow a boundary point

an observation point outside the system

a source point inside the system

proved by considering the Schrodinger equations obeyed by the two Green's functions involved, multiplying each equation by the other function and subtracting, obtaining a vanishing divergence, and invoking Gauss' theorem with respect to an appropriate boundary, using Dirichlet b.c. of the appropriate Green's function.

This is an integro-differential equation, relating the outgoing wave Green's function of the system at an external point, to its boundary value. The desired resonance b.c. is obtained by letting \mathbf{r} approach the boundary from outside and expanding the LHS in distance from the boundary. For simple geometries, the resulting expression degenerates into a Robin-like b.c.

AVERAGED DENSITY OF RESONANCES

- For a given realization of disorder, the resonance spectrum is a set of points in the complex energy plane $\zeta = \frac{\hbar^2 k^2}{2m}$ (on the unphysical sheet).
- We shall actually work with the complex momentum variable k, in which case resonances live in the 4th quadrant.
- They are poles of the resolvent

$$(\zeta, \zeta^*) = \operatorname{Tr} \frac{1}{\zeta - H_{eff}}$$

G(

- For a large system, these resonances will occupy a dense, two-dimensional region in the complex plane, rendering the resolvent nonanalytic in that region.
- Since the system is disordered, we are interested in averaging the density of resonances (DOR) over disorder.

Example - the resonance spectrum of a disordered chain



FIG. 4: Scatter plot for the case of strong disorder. The coupling strength η is taken to be 0.64. 1000 realizations for the matrix of size N = 1000 have been taken for W = 1.0.

Next we consider the case (*ii*) where $\xi > N$. In Fig. 7 we show the scatter plot ($\Re\{E\}$ vs $\Im\{E\}$) for weak disorder where W = 0.25, $\eta = 0.81$, N = 500 and the number realizations is 100. In Figs. 8 and 9, we show results for different values of W and N so that $\xi(0)/N = 3.2$. We have again chosen the uniform disorder with widths $W = 0.5, 0.5/\sqrt{2}$ and 0.25 for N = 125, 250 and 500 respectively. In Fig. 8 we show the average position of level vs percentage of levels below it for $\eta = 0.81$. As shown in the figure, these curves nearly overlap when $\Im\{E\}$ is scaled by N. Fig. 9 is the repetition of Fig. 8 for $\eta = 1.0$.

NUMERICAL RESULTS: SMALL η /STRONG DISORDER

THE SUPERSYMMETRIC METHOD

Efetov, Brezin (here I follow Verbaarschot)

A. Hermitian Case:

Hermitian hamiltonian H , real eigenvalues λ_i Quantity of interest:

$$F(z,w) = \frac{\det(z-H)}{\det(w-H)} = \prod_{i} \frac{(z-\lambda_i)}{(w-\lambda_i)}$$

$$F(z,z) = 1$$

23

Basic identity:
$$\frac{\partial}{\partial z}F(z,w) = F(z,w)\operatorname{tr}\frac{1}{z-H}$$

then
$$G(z) = \lim_{w \to z} \frac{\partial}{\partial z} F(z, w) = \sum_{i} \frac{1}{z - \lambda_i} = \operatorname{tr} \frac{1}{z - H}$$

G(z) is the resolvent of H

density of states:

$$\rho(x) = \sum_{i} \delta(x - \lambda_i) = \frac{1}{\pi} \operatorname{Im} G(x - i0)$$

generated by gaussian integration over Grassmann (anticommuting) variables

$$F(z, w) = \frac{\det(z - H)}{\det(w - H)}$$

generated by gaussian integration over bosonic (commuting) variables

bosonic integration

bosonic variables ϕ_i, ϕ_i^* $i = 1, \cdots, N$

$$\int \prod_{i} \frac{d^2 \phi_i}{\pi} \exp\left[i\phi^{\dagger}(z-H)\phi\right] = \frac{i^N}{\det(z-H)}, \quad \text{Im}z > 0$$

$$\int \prod_{i} \frac{d^2 \phi_i}{\pi} \exp\left[-i\phi^{\dagger}(z-H)\phi\right] = \frac{(-i)^N}{\det(z-H)}, \quad \text{Im}z < 0$$

integrals exists because H is hermitian

Expect trouble if H is nonhermitian with complex eigenvalues !

Berezin integration over Grassmann variables ψ_i, ψ_i^* $\{\psi_i, \psi_j^*\} = \{\psi_i, \psi_j\} = 0$





IT FOLLOWS THAT

$$\int \prod_{i} [d\psi_{i} d\psi_{i}^{*}] \exp\left[\pm i\psi^{\dagger}(z-H)\psi\right] = \left(\frac{\mp i}{\pi}\right)^{N} \det(z-H)$$

hence

$$\int \prod_{i} [d\psi_i d\psi_i^* d^2 \phi_i] \exp\left[\pm i\psi^{\dagger}(z-H)\psi \pm i\phi^{\dagger}(w-H)\phi\right] = \frac{\det(z-H)}{\det(w-H)}$$

NONHERMITIAN HAMILTONIAN - DIVERGING BOSONIC INTEGRALS !

for example $\int d^2 \phi e^{i\phi^*(z-z_0)\phi}$

won't converge if $\operatorname{Im}(z-z_0) > 0$

thus,
$$\int \prod_{i} d^{2} \phi_{i} e^{i\phi^{\dagger}(z-H)\phi}$$
would not make any sense once

 $z > \inf \operatorname{Im} \sigma(H)$

CONTRARY TO THIS,

$$f(z, z_0; \eta) = \int d^2 u d^2 d \exp\left[i(u^*, d^*) \left(\begin{array}{cc} \eta & z - z_0 \\ (z - z_0)^* & \eta \end{array}\right) \left(\begin{array}{c} u \\ d \end{array}\right)\right] = \frac{-\pi^2}{\eta^2 - |z - z_0|^2}$$

exists for all values of z, provided $\text{Im } \eta > 0$ in particular $f(z, z_0; 0) = \frac{\pi^2}{|z - z_0|^2}$

WE ARE THUS LED TO APPLY THE **METHOD OF HERMITIZATION:**

- by this method we reduce the problem of finding the eigenvalues of a nonhermitian operator to the more familiar problem of diagonalizing a hermitian one.
- have to double the vector space
- eigenvalues of the hermitian operator are essentially the singular values of the original nonhermitian operator.

given the nonhermitian operator H, we are led to consider the hermitian one

$$\mathcal{H} = \begin{pmatrix} 0 & z - H \\ (z - H)^{\dagger} & 0 \end{pmatrix}$$

this operator has chiral structure.

the chiral matrix $\Gamma_5 = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix} = \mathbf{1} \otimes \sigma_3$

anti-commutes with \mathcal{H} : $\{\mathcal{H}, \Gamma_5\} = 0$

thus, if is an eigenvector of \mathcal{H} with eigenvalue λ_{α} , $\mathcal{H}\xi_{\alpha} = \lambda_{\alpha}\xi_{\alpha}$

then $\Gamma_5 \xi_{\alpha}$ is an eigenvector with eigenvalue $-\lambda_{\alpha}$

in other words, nonzero eigenvalues of \mathcal{H} come in pairs $\pm \lambda_{\alpha}$

lower block of ξ_{α} is an eigenvalue of $(z - H)^{\dagger}(z - H)$ with eigenvalue λ_{α}^2 etc thus

$$\det \left(\begin{array}{cc} 0 & z-H \\ (z-H)^{\dagger} & 0 \end{array} \right) = \prod_{\lambda_{\alpha}>0} (-\lambda_{\alpha}^2) = (-1)^N \det \left[(z-H)^{\dagger} (z-H) \right]$$

thus, we shall use the Supersmmetric Method to generate the ratio of determinants

$$\mathcal{Z}(0) = \frac{\det \ ' \left(\begin{array}{cc} 0 & z - H \\ (z - H)^{\dagger} & 0 \end{array} \right)}{\det \ ' \left(\begin{array}{cc} 0 & w - H \\ (w - H)^{\dagger} & 0 \end{array} \right)} = \frac{|\det \ '(z - H)|^2}{|\det \ '(w - H)|^2}$$

 $\equiv |F(z,w)|^2$

now, by analiticity with respect to z, $\partial_z |F(z,w)|^2 = |F(z,w)|^2 \frac{\partial_z F(z,w)}{F(z,w)}$

and in the limit,

$$\lim_{w \to z} \partial_z |F(z,w)|^2 = \operatorname{Tr} \frac{1}{z-H}$$

as before.

At all stages of the calculation, all integrals are well defined and converge.

a doublet of complex bosonic fields: $\begin{pmatrix} u(\mathbf{r}) \\ d(\mathbf{r}) \end{pmatrix}$

 $d(\mathbf{r})$ is acted upon by H_{eff} . Hence this field is subjected to the resonance b.c. at the open boundary

 $u(\mathbf{r})$ is acted upon by H_{eff}^{\dagger} . Hence this field is subjected to the complex conjugated resonance b.c. at the open boundary

with these b.c.'s on the fields, $\mathcal{H} = \begin{pmatrix} 0 & w - H_{eff} \\ (w - H_{eff})^{\dagger} & 0 \end{pmatrix}$

is a self-adjoint operator in the volume of the system Ω

similarly, a doublet of complex fermionic fields:

$$\left(\begin{array}{c} \alpha({f r}) \\ \beta({f r}) \end{array}
ight)$$

 $\beta(\mathbf{r})$ is acted upon by H_{eff} . Hence this field is subjected to the resonance b.c. at the open boundary

 $\alpha(\mathbf{r})$ is acted upon by H_{eff}^{\dagger} . Hence this field is subjected to the complex conjugated resonance b.c. at the open boundary

with these b.c.'s on the fields,

$$\mathcal{H} = \begin{pmatrix} 0 & z - H_{eff} \\ (z - H_{eff})^{\dagger} & 0 \end{pmatrix}$$

is a self-adjoint operator in the volume of the system Ω

SUPERSYMMETRIC ACTION

$$\mathcal{L} = (u^*(\mathbf{r}), d^*(\mathbf{r})) \begin{pmatrix} \eta & w - H_{eff} \\ (w - H_{eff})^{\dagger} & \eta \end{pmatrix} \begin{pmatrix} u(\mathbf{r}) \\ d(\mathbf{r}) \end{pmatrix} +$$

$$(\alpha^*(\mathbf{r}), \beta^*(\mathbf{r})) \begin{pmatrix} \eta & z - H_{eff} \\ (z - H_{eff})^{\dagger} & \eta \end{pmatrix} \begin{pmatrix} \alpha(\mathbf{r}) \\ \beta(\mathbf{r}) \end{pmatrix}$$

action
$$S = \int_{\Omega} \mathcal{L} d\mathbf{r}$$

fermion-boson symmetry is precise when z=w. We shall always assume a smal z-w, which will slightly break SUSY (like a weak magnetic field in the Ising model) lump all fields into a single superfield:

$$(\mathbf{r}) = egin{pmatrix} u(\mathbf{r}) \ d(\mathbf{r}) \ lpha(\mathbf{r}) \ lpha(\mathbf{r}) \ eta(\mathbf{r}) \ eta(\mathbf{r}) \ eta(\mathbf{r}) \ eta(\mathbf{r}) \ eta(\mathbf{r}) \end{pmatrix}$$

Φ

define
$$\zeta = \frac{z+w}{2}, \Delta = \frac{z-w}{2}$$

then
 $\mathcal{L} = \Phi^{\dagger} \begin{bmatrix} \begin{pmatrix} \eta & \zeta - H_{eff} \\ (\zeta - H_{eff})^{\dagger} & \eta \end{bmatrix} \otimes \mathbf{1}_2 - \begin{pmatrix} 0 & \Delta \\ \Delta^* & 0 \end{bmatrix} \otimes \sigma_3 \end{bmatrix} \Phi$
the 2x2 matrices act on the fermion-boson blocks
they are diagonal, and therefore do not mix F and B
the last term, clearly breaks B-F symmetry when $\Delta \neq 0$

(i.e., $w \neq z$,). is therefore the small "magnetic field" alluded to above 40

Finally,

$$\mathcal{Z}(\eta) = \int_{rbc,\Omega} \mathcal{D}\Phi \mathcal{D}\Phi^{\dagger} e^{iS}$$

The desired (yet-to-be averaged) resolvent is obtained as

Tr
$$\frac{1}{z - H_{eff}} = \lim_{\eta \to +i0} \lim_{w \to z} \partial_z \mathcal{Z}(\eta)$$

- yet to average over Gaussian disorder potential V(r)
- this will produce quartic superfield self interaction.
- to cope with these, introduce supermatrix auxiliary fields, and use Hubbard-Stratonovich (complete squares) to disentangle the quartic term.
- superfields then appear quadratically in the action, and are integrated over, to produce an effective action for the supermatrix fields. These are then analysed under certain approximations...

THE END