Rigorous Aspects of a Simplified Polaron Model

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Abstract

In this research we studied various mathematical aspects of an interacting quantum system consisting of a free particle interacting with a field of spins. We first showed for a max of 2 spins the existence of low energy eigenvalues representing bounded solutions. Then for the infinite system, we showed the existence of low energy solutions which in physics literature is often called the polaron. We also obtained bounds for the effective mass of the interacting particle in terms of the specified parameters, which are the local potential as well as the interaction rate.

1 Introduction

In our model, the particle remembers the position and order of the spins it flips up, allowing a particle to only flip down the most recent spin it flipped up. This means the up spin locations are simply an ordered k-tuple in which $m_i \neq m_{i-1}$ for $i = 1, \cdots k$. Thus our system describes a tree-like graph of infinite copies of $\mathbb{Z}$ such that every point on $\mathbb{Z}$ contains a connection to another copy of $\mathbb{Z}$ with a different associated energy U. Additionally, the interaction rate between the field of spins and the particle is g. We can now describe the system by a function of the particle's position, and the up spin locations. Such a vector looks like

$$\Psi(n, A) = \begin{pmatrix} \psi_0(n) \\ \psi_1(n, m) \\ \psi_2(n, (m_1, m_2)) \\ \vdots \end{pmatrix}.$$

Here A is the ordered k-tuple of up spin positions with the last item in the tuple being the most recent spin particle that was flipped up. This system behaves in reaction to a discrete

Hamiltonian, which encodes all the interactions. This Hamiltonian when applied to $\Psi(n, A)$ gives us

$$\hat{H}\Psi(n,A) = -\begin{pmatrix} \psi_0(n+1) + \psi_0(n-1) \\ \psi_1(n+1,m) + \psi_1(n-1,m) \\ \psi_2(n+1,(m_1,m_2)) + \psi_2(n-1,(m_1,m_2)) \\ \vdots \end{pmatrix}$$

$$-\, g \begin{pmatrix} \psi_1(n,n) \\ \psi_0(n)I[n=m] + I[n \neq m]\psi_2(n,(m,n)) \\ \psi_1(n,m_1)I[n=m_2] + I[n \neq m_2]\psi_3(n,(m_1,m_2,n)) \\ \vdots \end{pmatrix} + \begin{pmatrix} 0 \\ U\psi_1(n,m) \\ 2U\psi_2(n,(m_1,m_2)) \\ \vdots \end{pmatrix}$$

We now desire to solve the eigenvalue equation for this system in order to understand and investigate the spectrum of the operator $\hat{H}$.

2 Transform

To simplify the situation we have to look at it becomes useful to make a transformation of the model by guessing a solution form of

$$\Phi = \begin{pmatrix} e^{ipn}\phi_0 \\ e^{ipm}\phi_1(m-n) \\ e^{ipm_1}\phi_2(m_1-n, m_2-n) \\ \vdots \end{pmatrix}.$$

Doing so turns us into a situation in which we look at all the spins relative to the location of the particle. Substituting this into the hamiltonian given in the intro we can do a change of variables to find a modified operator $\tilde{H}$ which we can linearly map back to our original operator, while solving the simpler form of our problem. This becomes

$$
\begin{aligned}
\tilde{H}\Phi = -&\begin{pmatrix} 2\cos(p) \\ \phi_1(m+1)+\phi_1(m-1) \\ \psi_2(m_1,m_2+1)+\phi_2(m_1,m_2-1) \\ \vdots \end{pmatrix} \\
&- g\begin{pmatrix} \phi_1(0) \\ \phi_0 I[m=0]+I[m\neq 0]\phi_2(m,0)) \\ \phi_1(m_1)I[m_2=0]+I[m_2\neq 0]\phi_3(m_1,m_2,0) \\ \vdots \end{pmatrix} + \begin{pmatrix} 0 \\ U\phi_1(m) \\ 2U\phi_2(m_1,m_2) \\ \vdots \end{pmatrix}.
\end{aligned}
$$

Now our requirement on $(m_1, \cdots, m_k)$ is simply that $m_i \neq 0$ for $i = 1, \cdots k-1$. Additionally all m_i before m_k tell us the direction that was moved on that layer of $\mathbb{Z}$ to the location a spin was created. It should be noted that this gives the graph a self similarity up to a shift of U as we move around it. This will become useful as we begin to look for low energy bound states to the original problem.

3 2nd Level Truncation

Truncating the main problem to allow for only two spins being up at one time we can attempt to understand the hierarchical model.

3.1 2-polaron Solution

First we want to find the 2-polaron solution which is represented by expotential decay on all layers above a constant 1 on the first layer. Thus

$$
\begin{pmatrix} f_0 \\ f_1 \\ f_2 \end{pmatrix} = \begin{pmatrix} 1 \\ ce^{-q|m|} \\ de^{-k|m_2|} \end{pmatrix}
$$

Applying to the Hamiltonian at position $m = 0$ we get the equations,

$$
\begin{aligned}
E &= -2e^{-q} - \frac{g}{c} + U \\
E &= -2\cos(p) - gc.
\end{aligned}
$$

Combing these two expressions gives us

$$e^{-q} = \frac{U-E}{2} + \frac{g^2}{2E+4\cos(p)}.$$

Now we look at a position m with $m_2 = 0$ and we can doe some algebra to show that

$$-2\cosh(q) = U - 2\cosh(k) - \frac{g^2}{2\sinh(k)}$$

In the 2-polaron situation. We now make some substitutes to find find a relation for k in terms of p.

$$(\frac{g^2}{2\sinh(k)} + \cosh(k) - \frac{U}{2}) - \frac{g^2}{4(U+\cos(p)-\cosh(k))} - \frac{U+\cos(p)-\cosh(k)}{(\cosh(k)-\frac{U}{2})(U+\cos(p)-\cosh(k))+\frac{g^2}{4}} = 0$$

To digest this expression a little easier we can define $V = U - 2\cosh(k)$ and $\tilde{V} = U - \cosh(k)$, then we end up with

$$\frac{g^2}{\sinh(k)} = V + \frac{g^2}{2(\tilde{V}+\cos(p))} - \frac{4(\tilde{V}+\cos(p))}{V(\tilde{V}+\cos(p)) - \frac{g^2}{2}}. \tag{1}$$

We will also find it useful to look at equation 1 in terms of U and E. Note that $V = E - U$ and $\tilde{V} = E/2$. Substituting into equation 1 and noting that $\sinh(k) = \sqrt{\cosh(k)^2 - 1}$ we have

$$0 = E - U + \frac{g^2}{(E+2\cos(p))} - \frac{4(E+2\cos(p))}{(E-U)(E+2\cos(p)) - g^2} - \frac{g^2}{\sqrt{(U-E/2)^2-1}}. \tag{2}$$

Using equation 2 we can prove the existence of solutions for E for p and U. This in turn suffices to prove the existence of k which are solutions to equation 1. However, in order to have physically valid solutions we need $e^{-q|m|}$ to be exponentially decaying. Thus $|e^{-q}| < 1$. Redefining $e^{-q} = Z(E)$ function we have

$$Z(E) = \frac{U-E}{2} + \frac{g^2}{2(E+2\cos(p))}.$$

Notice using this equation we can rewrite equation 2 in a more useful way as

$$0 = (E-U) + Z(E) + \frac{1}{Z(E)} + \frac{g^2}{\sqrt{(2U-E)^2-4}}. \tag{3}$$

To prove the existence of a solution to 1 we examine the singularities. We must first find regions in which $Z(E) = \pm 1$, since only energy values in this region will yield proper solutions for the 2-polaron. Setting $Z(E_{\pm\pm}) = \pm 1$, we use the quadratic equation to find that

$$E_{\pm\pm} = -\cos p + \frac{U}{2} \pm 1 \pm \sqrt{(-\cos p - \frac{U}{2} \mp 1)^2 + g^2} \tag{4}$$

This yields 4 unique values of E,

$$\begin{aligned}
E_{--} &= -\cos p + \frac{U}{2} - 1 - \sqrt{(-\cos p - \frac{U}{2} + 1)^2 + g^2} \\
E_{-+} &= -\cos p + \frac{U}{2} - 1 + \sqrt{(-\cos p - \frac{U}{2} + 1)^2 + g^2} \\
E_{+-} &= -\cos p + \frac{U}{2} + 1 - \sqrt{(-\cos p - \frac{U}{2} - 1)^2 + g^2} \\
E_{++} &= -\cos p + \frac{U}{2} + 1 + \sqrt{(-\cos p - \frac{U}{2} - 1)^2 + g^2}.
\end{aligned}$$

Where $Z(E_{--}) = Z(E_{-+}) = 1$ and $Z(E_{+-}) = Z(E_{++}) = -1$.

Theorem 1. *Let $E_{\pm\pm}$ be defined as in equation 4 above and $U \geq 4$, then $E_{--} \leq E_{+-} \leq E_{-+} \leq E_{++}$.*

Proof. To show that $E_{-+} \leq E_{++}$, set $A = -\cos p$ and $B = \frac{U}{2}$. Notice, $E_{\pm\pm} = A + B \pm 1 \pm \sqrt{(B - A \pm 1)^2 + g^2}$. Then,

$$\begin{aligned}
E_{-+} &= A + B - 1 + \sqrt{(B - A - 1)^2 + g^2} \\
E_{++} &= A + B + 1 + \sqrt{(B - A + 1)^2 + g^2}
\end{aligned}$$

Notice that as $U \geq 4$ we have that $B - A = \frac{U}{2} + \cos p \geq 0$ for all p. Additionally, we have that $B - A = -\cos p + \frac{U}{2} \geq 0$ for all p. Then, $B - A + 1 \geq B - A - 1$ and thus, $(B - A + 1)^2 \geq (B - A - 1)^2$. It follows that

$$\sqrt{(B - A + 1)^2 + g^2} \geq \sqrt{(B - A - 1)^2 + g^2}$$

Also, we have $A + B - 1 \leq A + B + 1$. It then is clear that $E_{-+} \leq E_{++}$. To prove $E_{+-} \leq E_{-+}$, notice that:

$$\begin{aligned}
E_{+-} = A + B + 1 - \sqrt{(B - A + 1)^2 + g^2} &\leq A + B + 1 - \sqrt{(B - A + 1)^2} \\
&\leq A + B + 1 - (B - A + 1) \\
&\leq 2A \\
&\leq -2\cos p
\end{aligned}$$

We also have,

$$\begin{aligned}
E_{-+} = A + B - 1 + \sqrt{(B-A-1)^2 + g^2} &\geq A + B - 1 + \sqrt{(B-A-1)^2} \\
&\geq A + B - 1 + (B - A + 1) \\
&\geq 2B \\
&\geq U
\end{aligned}$$

By our assumption that $U > 4$, we have that $U > -2\cos p$ and thus, $E_{+-} \leq E_{-+}$. It remains to be shown that $E_{--} \leq E_{+-}$. □

Now we prove the existence of solutions for the 2-polaron. We can use equation 3 to give us a function $S(E)$ where

$$S(E) = (E - U) + Z(E) + \frac{1}{Z(E)} + \frac{g^2}{\sqrt{(2U-E)^2 - 4}}.$$

We already know by definition that $Z(E_{--}) = 1$ and $Z(E_{+-}) = -1$. The only valid solutions to the 2-polaron will come into play for E_r's such that $E_r \in (E_{--}, E_{+-})$ and $S(E_r) = 0$. We know that $Z(E_-) = 0$ and $E_- \in (E_{--}, E_{+-})$. This tells us that somewhere to the right of E_{--} in our allowed interval $S(E)$ will shoot to positive infinity. Therefore, it suffices to prove the existence of a solution by proving that $S(E_{--}) < 0$ for some values of U, g, and p.

Theorem 2. *Let $U > 6$, $p \in \mathbb{R}$, and $g > 0$, then $S(E_{--}) < 0$.*

Proof. Define $A = -U/2 - \cos(p)$. Because $6 < U$, we see that $A < -2 < 0$. Notice

$$g = |g| = \sqrt{g^2} < \sqrt{(A+1)^2 + g^2},$$

since $A + 1 \neq 0$. Therefore

$$E_{--} = A + U - 1 - \sqrt{(A+1)^2 + g^2} < A + U - g.$$

Now we also can see that

$$2U - E_{--} > U + g - A > 6 + g - A > 0.$$

Since $2U - E_{--}$ and $g - A + 6$ are positive, we know $(2U - E_{--})^2 > (g - A + 6)^2$. From this we can see that $\sqrt{(2U - E_{--})^2 - 4} > \sqrt{(g - A + 6)^2 - 4} > g - A > 0$. Hence

$$\frac{g^2}{\sqrt{(2U - E_{--})^2 - 4}} < \frac{g^2}{g - A} < g.$$

From all of these relations we can now see that

$$\begin{aligned} S(E_{--}) &= (E_{--} - U) + 1 + 1 + \frac{g^2}{\sqrt{(2U-E)^2-4}} \\ &< A - g + 2 + \frac{g^2}{\sqrt{(2U-E)^2-4}} \\ &< A - g + 2 + \frac{g^2}{g-A} \\ &< A - g + 2 + g \\ &< 0. \end{aligned}$$

$\square$

Now we see that by Theorem 2 the 2-polaron solution exists for all p and $g > 0$ whenever we have at least $U > 6$. This ends our investigation of the truncated model. While we believe better bounds exist, for now we want to move on and consider the full model by not allowing limits to our up-spins.

4 Full-Model Polaron Solution

We now want to understand the low energy polaron solution to the full model and will seek to prove the existence and some behavior of it in this section. We can define $\phi_0 = 1$ as a free choice of ours for this solution. Doing so gives us

$$\Phi = \begin{pmatrix} 1 \\ \phi_1(m_1) \\ \phi_2(m_1, m_2) \\ \vdots \end{pmatrix} = \begin{pmatrix} 1 \\ \Phi_m \end{pmatrix}. \tag{5}$$

Now we can rewrite our Hamiltonian operator as a matrix in the following manner

$$\tilde{H} = \begin{pmatrix} -2\cos(p) & -g\hat{F}^T & 0 & 0 & 0 & \cdots \\ -g\hat{F} & \hat{H}_1 & -g\hat{F}^T & 0 & 0 & \cdots \\ 0 & -g\hat{F} & \hat{H}_2 & -g\hat{F}^T & 0 & \cdots \\ \vdots & & \ddots & & & \ddots \end{pmatrix} = \begin{pmatrix} -2\cos(p) & -g\tilde{F}^T \\ -g\tilde{F} & \mathcal{H} \end{pmatrix}. \tag{6}$$

Where $\hat{F}\phi_i(m_1, \cdots, m_i) = \phi_i(m_1, \cdots, m_i)\delta_0(m_{i+1})$ and $\hat{F}^T\phi_i(m_1, \cdots, m_i) = \phi_i(m_1, \cdots, m_{i-1}, 0)$. Additionally, $\hat{H}_k\phi_i(m_1, \cdots, m_i) = -\phi_i(m_1, \cdots, m_i+1) - \phi_i(m_1, \cdots, m_i-1) + kU\phi_i(m_1, \cdots, m_i)$.

$\tilde{F}$ and $\tilde{F}^T$ are defined similarly but modified to adjust the dimension of the vectors they eat and return. It should be clear how this alternate definition matches the previously stated definition of $\tilde{H}$. We claim there is an E range in which we can invert $\mathcal{H} - E$.

Lemma 1. *The operator $\mathcal{H} - E$ for some $E \in \mathbb{R}$ is invertible at least on the interval $(-\infty, U - 2 - 2g)$.*

Proof. Let $\mathcal{H}$ and Φ_m be defined as in equations 6 and 5 respectively. Throughout this proof we will also write $\phi_k(m_1, \cdots, m_k) = \phi_k(m_k)$ in order to save space, however note all phi_k are functions of k variables. It suffices to show that $\langle \Phi_m | \mathcal{H} \Phi_m \rangle \geq -2||\Phi_m||^2 - 2g||\Phi_m||^2 + U||\Phi_m||^2$ in order to prove this Lemma. Let us rewrite $\mathcal{H} = \mathcal{H}_U + \mathcal{H}_h + \mathcal{H}_g$ which are operators for the local potential, side to side hopping, and the g interaction terms respectively. First notice

$$\langle \Phi_m | \mathcal{H}_U \Phi_m \rangle = \sum_{k=1}^{\infty} \sum_{(m_1, \cdots, m_k)} \phi_k^*(m_k)[kU\phi_k(m_k)] \geq U \sum_{k=1}^{\infty} \sum_{(m_1, \cdots, m_k)} |\phi_k(m_k)|^2 = U||\Phi_m||^2.$$

Now see that

$$\begin{aligned}
\frac{\langle \Phi_m | \mathcal{H}_g \Phi_m \rangle}{-g} &= \sum_{k=1}^{\infty} \sum_{(m_1, \cdots, m_k)} \phi_k^*(m_k)[\hat{F}^T \phi_k(m_k) + \hat{F}\phi_k(m_k)] - \sum_{m_1} \phi_1^*(m_1)\hat{F}^T \phi_1(m_1) \\
&\leq \sum_{k=1}^{\infty} \sum_{(m_1, \cdots, m_k)} \phi_k^*(m_k)[\phi_k(0) + \phi_k(m_k)\delta_0(m_{k+1})] \\
&\leq 2 \sum_{k=1}^{\infty} \sum_{(m_1, \cdots, m_k)} |\phi_k(m_k)|^2 \\
&= 2||\Phi_m||^2.
\end{aligned}$$

From this we see that $\langle \Phi_m | \mathcal{H}_g \Phi_m \rangle \geq -2g||\Phi_m||^2$. Finally, we look at $\mathcal{H}_h$. We find here how

$$\begin{aligned}
\langle \Phi_m | \mathcal{H}_g \Phi_m \rangle &= \sum_{k=1}^{\infty} \sum_{(m_1, \cdots, m_k)} \phi_k^*(m_k)[-\phi_k(m_k + 1) - \phi_k(m_k)] \\
&= \frac{1}{2} \sum_{k=1}^{\infty} \sum_{(m_1, \cdots, m_k)} |\phi_k(m_k) - \phi_k(k_k + 1)|^2 + |\phi_k(m_k) - \phi_k(m_k - 1)|^2 \\
&\qquad\qquad - 2|\phi_k(m_k)|^2 - |\phi_k(m_k + 1)|^2 - |\phi_k(m_k - 1)|^2 \\
&= \sum_{k=1}^{\infty} \sum_{(m_1, \cdots, m_k)} |\phi_k(m_k) - \phi_k(m_k + 1)|^2 - 2|\phi_k(m_k)|^2 \\
&\geq -2||\Phi_m||.
\end{aligned}$$

Since the inner product operator is linear we are left with $\langle \Phi_m | \mathcal{H} \Phi_m \rangle \geq -2||\Phi_m||^2 - 2g||\Phi_m||^2 + U||\Phi_m||^2$. Thus if $E < U - 2 - 2g$ we know $\mathcal{H} - E$ is invertible. $\square$

From Lemma 1 we now know we can talk about $(\mathcal{H} - E)^{-1}$ for some E regime. We want to now show the analyticity of this operator when applied to a vector so we can show the ability to differentiate it in E.

Lemma 2. *The operator $F(E) = (\mathcal{H} - E)^{-1}\psi$ is real analytic for some interval and $(\mathcal{H} - E)^{-1}$ acts like the inverse of $(\mathcal{H} - E)$ on that interval.*

Proof. Let $F(E) = (\mathcal{H} - E)^{-1}\psi$. By Lemma 1 we know we can invert $(\mathcal{H} - E)$ on $(-\infty, U - 2 - 2g)$. So choose some $E \in (-\infty, U - 2 - 2g)$. We now know $||(\mathcal{H} - E)^{-1}|| < \infty$. Thus we can find some w such that $||(\mathcal{H} - E)^{-1}|| \cdot ||w|| < 1$. See that

$$\begin{aligned} \frac{1}{\mathcal{H} - (E + w)} = \frac{1}{(\mathcal{H} - E) - w} &= \frac{1}{H - E} \cdot \frac{1}{1 - \frac{w}{H - E}} \\ &= \sum_{n=0}^{\infty} w^n (\mathcal{H} - E)^{-n-1}. \end{aligned}$$

By definition of w then we know $\sum_{n=0}^{\infty} w^n (\mathcal{H} - E)^{-n-1}\psi$ converges for our chosen E. Now see that

$$\begin{aligned} (\mathcal{H} - (E + w)) \sum_{n=0}^{\infty} w^n (\mathcal{H} - E)^{-n-1} &= w\Big(\sum_{n=0}^{\infty} w^{n-1} (\mathcal{H} - E)^{-n} - \sum_{n=0}^{\infty} w^n (\mathcal{H} - E)^{-n-1} \Big) \\ &= w\Big(\frac{1}{w} - (\mathcal{H} - E)^{-1} + (\mathcal{H} - E)^{-1} - \cdots \Big) \\ &= 1. \end{aligned}$$

So $(\mathcal{H} - E)^{-1}$ does act as an inverse in some neighborhood of our chosen E. From all of this it follows that $F(E)$ is analytic for some neighborhood of $E \in (-\infty, U - E - 2g)$. This tells us that we would expect to see errors in $F(E)$ whenever we either approach singularities, or branch points. $\square$

Now we want to imagine cutting off our connection to the bottom transformation layer. At $m_1 = 0$ then we are simply left with some vector δ_0 and no connection to ϕ_0. In this picture then $\mathcal{H}$ is self similar to itself, this allows us to easily rewrite $\mathcal{H}$ in the same way we rewrote $\tilde{H}$. That is

$$\mathcal{H} = \begin{pmatrix} \hat{H}_1 & -g\tilde{F}^T \\ -g\tilde{F} & \mathcal{H} + U \end{pmatrix}. \tag{7}$$

Applying this to some arbitrary vector we can find

$$\mathcal{H}\begin{pmatrix}\phi_1(m_1)\\ \Phi_r\end{pmatrix}=\begin{pmatrix}\hat{H}_1\phi_1(m_1)-g\tilde{F}^T\Phi_r-\delta_0(m_1)\\ -g\tilde{F}\phi_1(m_1)+(\mathcal{H}+U)\Phi_r\end{pmatrix}=E\begin{pmatrix}\phi_1(m_1)\\ \Phi_r\end{pmatrix}.$$

The second line allows us to obtain $\Phi_r=-g(\mathcal{H}+U-E)^{-1}\tilde{F}1\phi_1(m_1)$. By definition $\tilde{F}^T(H-E)^{-1}\tilde{F}1=\langle\delta_0|(H-E)^{-1}\delta_0\rangle$, thus we end with the equation

$$-(\phi_1(m_1+1)+\phi_1(m_1-1))-g^2I[m\neq 0]\langle\delta_0|(H-E+U)^{-1}\delta_0\rangle\phi_1(m_1)+(U-E)\phi_1(m_1)=\delta_0(m_1).$$

We are looking for bound state polaron solutions to our initial problem. Because of this the only form for our eigenfunctions must be $\phi_1(m_1)=ce^{-k|m_1|}$ since they need to decay in order to be physical. The equation above then will give us the relations that

$$-2\cosh(k)=g^2\langle\delta_0|(H-E+U)^{-1}\delta_0\rangle-U+E,$$

and

$$c=\frac{1}{-2e^{-k}+E-U}.$$

Therefore we arrive at

$$c=\frac{1}{g^2\langle\delta_0|(H-E+U)^{-1}\delta_0\rangle+2\sinh(k)}.$$

Notice that if we were to now include the bottom layer of our system we would find that $c=\langle\delta_0|(H-E)^{-1}\delta_0\rangle$. Thus defining $G(E)=\langle\delta_0|(H-E)^{-1}\delta_0\rangle$ and recalling $\sinh(x)^2=\cosh(x)^2-1$, we find that

$$G(E)=\frac{1}{g^2G(E-U)+\sqrt{(E-U+g^2G(E-U))^2-4}}. \tag{8}$$

Here $G(E)$ becomes our so called Green's function. Applying the same ideas to the eigenvalue equation of the operator from Equation 6 we find that

$$-g^2G(E_p)=E_p+2\cos(p), \tag{9}$$

is the equation we need to solve in order to get eigenvalues and eigenvectors for our whole model. Here quickly also notice that E_p is expected to depend on the value of p we choose.

4.0.1 Green's Function

We have now defined our Green's function as $G(E) = \langle \delta_0 | (\mathcal{H} - E)^{-1} \delta_0 \rangle$. We know as E begins to approach the spectrum of $\mathcal{H}$ then $G(E)$ will diverge to an infinity since $(\mathcal{H} - E)$ will cease to be invertible. We have the general bound that $\langle \Phi_m | \mathcal{H} \Phi_m \rangle \geq -2||\Phi_m||^2 - 2g||\Phi_m||^2 + U||\Phi_m||^2$. So we know there exists some $E_c > -\infty$ for which $(-\infty, E_c)$ is a interval where $G(E)$ is defined and Lemma 2 tells us we can differentiate in respect to E on this interval as well. We then desire to prove some behavior of $G(E)$ in order to better understand the existence of solutions to Equation 9.

Lemma 3. *G(E) is an increasing function of E.*

Proof. Let $G(E)$ be as so defined. We know that $\mathcal{H}$ is a hermitian operator and since E is an eigenvalue of $\mathcal{H}$, we have that $E \in \mathbb{R}$. Thus

$$\begin{aligned} \frac{d}{dE} G(E) &= \frac{d}{dE} \langle \delta_0 | (\mathcal{H} - E)^{-1} \delta_0 \rangle \\ &= \langle \delta_0 | (\mathcal{H} - E)^{-2} \delta_0 \rangle \\ &= \langle (\mathcal{H} - E)^{-1} \delta_0 | (\mathcal{H} - E)^{-1} \delta_0 \rangle \\ &= ||(\mathcal{H} - E)^{-1} \delta_0||^2 > 0. \end{aligned}$$

From this we can discern that $G(E)$ is an increasing function of E. $\square$

From Lemma 3 we can define the point E_{cr} to be where $g^2 G(E_{cr}) G(E_{cr} - U) = 1$. Notice here that E_{cr} will come before the spectrum of $\mathcal{H}$. Equation 8 further limits us to seeking a value for E in which $(E - U + g^2 G(E - U))^2 - 4$ is away from 0. Since we are coming from $-\infty$ for E we want to look at -2 first. See how if

$$E_{cr} - U + g^2 G(E_{cr} - U) = -2,$$

then $g^2 G(E_{cr}) G(E_{cr} - U) = 1$. Thus this is the exact value we mentioned before, which is well away form the spectrum of $\tilde{H}$. So we want to consider $G(E)$ on the interval $(-\infty, E_{cr})$, and seek to solve the equation $-g^2 G(E) = E + 2\cos(p)$.

Lemma 4. *$G(E)$ is bounded above by $\frac{1}{U-E-2}$ and below by $\frac{1}{U-E}$ on the interval $(-\infty, E_{cr})$.*

Proof. Let $g \in \mathbb{R}^+$. Notice that on the interval $(-\infty, E_{cr})$, we have $E-U+g^2G(E-U) < -2$. Hence,

$$\begin{aligned}
\frac{1}{G(E)} &= \sqrt{(E-U+g^2G(E-U)+2)(E-U+g^2G(E-U)-2)} + g^2G(E-U) \\
&\geq \sqrt{(E-U+g^2G(E-U)+2)^2} + g^2G(E-U) \\
&= |E-U+g^2G(E-U)+2| + g^2G(E-U) \\
&= U-E-g^2G(E-U)-2+g^2G(E-U) \\
&= U-E-2.
\end{aligned}$$

Thus

$$G(E) \leq \frac{1}{U-E-2}.$$

Next, for the lower bound we can apply the arithmetic geometric mean inequality See that

$$\begin{aligned}
\frac{1}{G(E)} &= \sqrt{(E-U+g^2G(E-U)+2)(E-U+g^2G(E-U)-2)} + g^2G(E-U) \\
&\leq \frac{|E-U+g^2G(E-U)-2|}{2} + \frac{|E-U+g^2G(E-U)+2|}{2} + g^2G(E-U) \\
&= \frac{U-E-g^2G(E-U)+2}{2} + \frac{U-E-g^2G(E-U)-2}{2} + g^2G(E-U) \\
&= U-E.
\end{aligned}$$

Therefore,

$$G(E) \geq \frac{1}{U-E},$$

hence, proved. □

Lemma 5. $\lim_{E\to-\infty} G(E) = 0$.

Proof. Let $G(E)$ be defined as in equation 8. It is obvious that

$$\lim_{E\to-\infty} \frac{1}{U-E-2} = 0,$$

and

$$\lim_{E\to-\infty} \frac{1}{U-E} = 0.$$

By Lemma 4 we know $\frac{1}{U-E-2}$ and $\frac{1}{U-E}$ bound $G(E)$ on $(-\infty, E_{cr})$. Hence

$$\lim_{E\to-\infty} G(E) = 0.$$

□

From Lemma 3 and 5 we get a quick corollary about $G(E)$.

Corollary 1. *$G(E) > 0$ on $(-\infty, E_{cr})$.*

Proof. Clear from Lemma 3 and 5. If $G(E) \leq 0$ for any $E \in (-\infty, E_{cr})$ then either $G(E)$ couldn't approach 0 as $E \to -\infty$ or $G(E)$ couldn't be increasing on that domain. $\square$

Lemma 6. *$G'(E) \geq G(E)^2$ on the interval $(-\infty, E_{cr})$.*

Proof. Let $p \in \mathbb{R}$ and let Γ be the graph that our model is defined on. Recall from the proof of Lemma 3 that $G'(E) = ||(\mathcal{H} - E)^{-1}\delta_0||^2$. Additionally, by definition

$$||(\mathcal{H} - E)^{-1}\delta_0||^2 = \sum_{x \in \Gamma} |[(\mathcal{H} - E)^{-1}\delta_0](x)|^2.$$

We know $\delta_0 \in \Gamma$, therefore

$$\begin{aligned} ||(\mathcal{H} - E)^{-1}\delta_0||^2 &\geq |[(\mathcal{H} - E)^{-1}\delta_0](\delta_0)|^2 \\ &= |\langle \delta_0, (\mathcal{H} - E)^{-1}\delta_0 \rangle|^2 \\ &= G(E)^2. \end{aligned}$$

Hence $G'(E) \geq G(E)^2$ on the interval $(-\infty, E_{cr})$, since $G(E) > 0$ on that interval. $\square$

Lemma 7. *The point E_{cr} is bounded above by $U - 2 + g$ and below by $U - 2 - g$ for all positive U and g.*

Proof. Let $U, g \in \mathbb{R}^+$. To prove these bounds, recall that Lemma 3 and Lemma 4 give us $G(E_{cr} - U) < G(E_{cr}) \leq (U - E_{cr} - 2)^{-1}$. Which we can rewrite as

$$\frac{U - E_{cr} - 2}{g^2} < \frac{1}{U - E_{cr} - 2}.$$

This gives us a quadratic relation in E_{cr} with a positive squared turn. Hence, E_{cr} will be bounded by the roots of the equation

$$(U - E_{cr} - 2)^2 - g^2 = 0.$$

Using the quadratic formula, we find

$$\begin{aligned} E_{cr} &= \frac{2U - 4}{2} \pm \frac{\sqrt{(4 - 2U)^2 - 16 + 16U + 4g^2 - 4U^2}}{2} \\ &= U - 2 \pm \sqrt{4 - 4U + U^2 - 4 + 4U + g^2 - U^2} \\ &= U - 2 \pm g \end{aligned}$$

Since $g > 0$ we conclude that $U - 2 - g < E_{cr} < U - 2 + g$. $\square$

Theorem 3. *The equation $-g^2G(E_p) = E_p + 2\cos(p)$ has solutions $E_s \in (-\infty, E_{cr})$, for all positive g and p whenever $U > 4$.*

Proof. Let $U > 4$ and let $g, p \in \mathbb{R}^+$. Since $G(E)$ is an increasing function of E by Lemma 3, we know $-g^2G(E)$ is decreasing in E on $(-\infty, E_{cr})$. Similarly $E + 2\cos(p)$ is an increasing function of E for all E. Therefore it suffices to show that $E_{cr} + 2\cos(p) + g^2G(E_{cr}) > 0$ to prove existence of some $E_s \in (-\infty, E_{cr})$ for which $-g^2G(E_s) = E_s + 2\cos(p)$. Recall that E_{cr} satisfies the relation that $E_{cr} - U + g^2G(E_{cr} - U) = -2$. Thus

$$G(E_{cr} - U) = \frac{U - E_{cr} - 2}{g^2}.$$

By equation 8 we can easily see that $G(E_{cr}) = (U - E_{cr} - 2)^{-1}$. By Lemma 3 and $U > 0$ we know $G(E - U) < G(E)$. Therefore

$$\frac{U - E_{cr} - 2}{g^2} < \frac{1}{U - E_{cr} - 2} \Rightarrow U - E_{cr} - 2 < g^2G(E_{cr}).$$

Hence $E_{cr} + 2\cos(p) + g^2G(E_{cr}) > E_{cr} + 2\cos(p) + U - E_{cr} - 2 = U - 2 + 2\cos(p)$. Finally then, because $U > 4$ we have $E_{cr} + 2\cos(p) + g^2G(E_{cr}) > 0$. Therefore a solution E_s must exist. □

Theorem 4. $E_{cr} + 2\cos(p) + g^2G(E_{cr}) \geq U - 2 + 2\cos(p) + \frac{g^2}{2} \cdot \frac{U+g}{U+2+g}$.

Proof. Let $G(E)$ be defined as normal, and $p \in \mathbb{R}$. Recall that $g^2G(E_{cr} - U) + E_{cr} - U = -2$. See that

$$\begin{aligned}
E_{cr} + 2\cos(p) + g^2G(E_{cr}) &= E_{cr} + 2\cos(p) + g^2G(E_{cr} - U) + g^2 \int_{E_{cr}-U}^{E_{cr}} G'(E)dE \\
&= U - 2 + 2\cos(p) + g^2 \int_{E_{cr}-U}^{E_{cr}} G'(E)dE \\
&\geq U - 2 + 2\cos(p) + g^2 \int_{E_{cr}-U}^{E_{cr}} G(E)^2 dE \quad \text{(Lemma 6)} \\
&\geq U - 2 + 2\cos(p) + g^2 \int_{E_{cr}-U}^{E_{cr}} \frac{1}{(U-E)^2} dE \quad \text{(Lemma 4)} \\
&= U - 2 + 2\cos(p) + g^2[\frac{1}{U - E_{cr}} - \frac{1}{U - (E_{cr} - U)}] \\
&= U - 2 + 2\cos(p) + g^2[\frac{1}{2} - \frac{1}{U + 2 + g}] \quad \text{(Lemma 7)} \\
&= U - 2 + 2\cos(p) + \frac{g^2}{2} \cdot \frac{U + g}{U + 2 + g}.
\end{aligned}$$

□

4.0.2 Effective Mass

We have now seen plenty of results on the existence of the low energy bound state solutions E_p. We now want to develop a bound on the effective mass of our system. By definition the effective mass is

$$\frac{1}{m_{eff}} = \frac{\partial^2}{\partial p^2} E_p \bigg|_{p=0}.$$

To find this we implicitly differentiate $-g^2 G(E_p) = E_p + 2\cos(p)$. See that

$$\begin{aligned} -g^2 G'(E_p) \frac{\partial E_p}{\partial p} &= \frac{\partial E_p}{\partial p} - 2\sin(p) \\ \Rightarrow \frac{\partial E_p}{\partial p} &= \frac{2\sin(p)}{1 + g^2 G'(E_p)}. \end{aligned}$$

From here it is a simple calculation to arrive at

$$m_{eff} = \frac{1}{2} + \frac{g^2}{2} G'(E_0). \tag{10}$$

Equation 10 is something we can quickly bound by applying Lemmas 6 and 4. See that

$$\begin{aligned} m_{eff} &= \frac{1}{2} + \frac{g^2}{2} G'(E_0) \\ &\geq \frac{1}{2} + \frac{g^2}{2} G(E_0)^2 \\ &\geq \frac{1}{2} + \frac{g^2}{2} \frac{1}{(2U - E_0)^2} \\ &\geq \frac{1}{2} + \frac{g^2}{2} \frac{1}{(U + g + 2)^2}. \end{aligned}$$

We would now like to use the Combes-Thomas bound on the Green's function to develop the upper bound on the effective mass. Doing so will take some more effort, and is part of the ongoing research we would like to continue after this program ends.

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