Rigorous Aspects of a Simplified Polaron Model

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1 Introduction

2 Definition's and Set Up

We want to provide a definition of the Hamiltonian we are investigating in this paper in formal grounds. This operator will be acting on a function that keeps track of a particles position and then a set of k-tuples which keep track of the locations of the up spins, as these are the only spins with associated energy. We can write this function out as

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

From here the particle will be effected by the points directly left and right of it on the level of $\mathbb{Z}$ it currently resides on, as well as the local energy at it's own point, and the connection to another layer of $\mathbb{Z}$. If the particle is at the position of the most recent spin, this connection looks down a layer, if we are at any other spot we can make a new spin up and move up a layer there. All this describes the following action from the operator on Ψ,

$$\hat{H}\Psi(n,A) = -\begin{pmatrix} \psi_0(n+1)+\psi_0(n-1) \\ \psi_1(n+1,m)+\psi_1(n-1,m) \\ \psi_2(n+1,(m_1,m_2))+\psi_2(n-1,(m_1,m_2)) \\ \vdots \end{pmatrix}$$
$$- g\begin{pmatrix} \psi_1(n,n) \\ \psi_0(n)I[n=m]+I[n\neq m]\psi_2(n,(m,n)) \\ \psi_1(n,m_1)I[n=m_2]+I[n\neq m_2]\psi_3(n,(m_1,m_2,n)) \\ \vdots \end{pmatrix} + \begin{pmatrix} 0 \\ U\psi_1(n,m) \\ 2U\psi_2(n,(m_1,m_2)) \\ \vdots \end{pmatrix}.$$

3 Proof of Theorem 1

Theorem 1. *Bound state solutions solving $-g^2G(E_p) = E_p + 2\cos(p)$ exist for all $p \in [-\pi,\pi)$ below the spectrum of $\mathcal{H}$ in the regimes of $U > 4$ and $g > 0$, or $g > \frac{2}{3}((27-3\sqrt{57})^{\frac{1}{3}} + (3(9+\sqrt{57}))^{\frac{1}{3}}) \approx 3.54$ and $U > 0$.*

Proof. First define $G(E) = \tilde{F}^T(\mathcal{H}-E)^{-1}\tilde{F}1 = \langle\delta_0|(\mathcal{H}-E)^{-1}\delta_0\rangle$. We begin by asserting that $G(E)$ is an analytic function of E on some real interval $(-\infty, E_c)$ where E_c is of now some unknown real number. The proof of this fact is given in the appendix, but is omitted here. We can now easily show some defining behavior of $G(E)$. The first is given by Lemma 1.

Lemma 1. *G(E) is an increasing function of E.*

Proof. 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 easily see that $G(E)$ is an increasing function of E. □

From Lemma 1 it immediately follows that $-g^2G(E)$ is a decreasing function of E. Similarly $E + 2\cos(p)$ is an increasing function of E. Therefore if we can show that at the boundary E_c in which $G(E)$ ceases to be well defined that $E_c + 2\cos(p) + g^2G(E_c) > 0$, we know solutions to $-g^2G(E_p) = E_p + 2\cos(p)$ must indeed exist. To this aim we seek to provide bounds on $G(E)$, E_c and as will become relevant $G'(E)$.

We first provide bounds for $G(E)$ on the interval $(-\infty, E_c)$ by appealing to the self consistent equation for $G(E)$.

Lemma 2. *$G(E)$ 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

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

Using the arithmetic geometric mean inequality we now seek to show the lower bound of $G(E)$ as follows

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

Therefore,

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

□

From Lemma 2 it is clear that as $E \to -\infty$ we must have that $G(E)$ approaches 0. When coupled with the fact that $G(E)$ is strictly increasing it is a simple result that $G(E) > 0$ for all $E \in (-\infty, E_c)$. The positivity of $G(E)$ is a useful fact that we will be using in various locations for the rest of the proof.

From this we can also prove a bound of $G'(E)$.

Lemma 3. *The point E_{cr} is bounded above by $U-2+g$ and below by $U-2$ for all positive U and g.*

Proof. Let $U, g \in \mathbb{R}^+$. To prove these bounds, recall that Lemmas 1 and 2 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

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

This is simply a difference of two squares, so we find

$$E_{cr} = U - 2 \pm g.$$

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

Lemma 4. $G'(E) \geq G(E)^2$ *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 1 that $G'(E) = ||(\tilde{H} - E)^{-1}\delta_0||^2$. Additionally, by definition

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

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

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

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

Lemma 5. $E_{cr} + 2\cos(p) + g^2 G(E_{cr}) \geq U - 2 + 2\cos(p) + \frac{g^2}{2} \cdot \frac{U+g}{U+2+g}$.

Proof. Let $G(E)$ be defined as normal, and $p \in \mathbb{R}$. Recall that $g^2 G(E_{cr}-U)+E_{cr}-U = -2$. See that, using Lemmas 4, 2, and 3,

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

□

Proof of Theorem 1 cont. Since $G(E)$ is an increasing function of E by Lemma 1, we know $-g^2 G(E)$ 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 $E_{cr} + 2\cos(p) + g^2 G(E_{cr}) > 0$ (the LHS of the Lemma 5 equation) to prove existence of some $E_s \in (-\infty, E_{cr})$ for which $-g^2 G(E_s) = E_s + 2\cos(p)$. Therefore, the RHS of the equation from Lemma 5 must be greater or equal to 0, which can always be the case with restrictions on U, g. If $U > 4$, g can be any positive number, and when $g > \frac{2}{3}((27 - 3\sqrt{57})^{\frac{1}{3}} + (3(9+\sqrt{57}))^{\frac{1}{3}}) \approx 3.54$, U can be any positive number. U, g can also both be less than $4, \approx 3.54$ if the RHS of the Lemma 5 equation is greater than 0. □

4 Appendix

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

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

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

Lemma 6. *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 2 and 1 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. □

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6 References