Preliminary notes from Houston visit # 1: 12.3.15 - 22.3.15.

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I. SOME MODELS

The Hamiltonian considered in LW is

$$H_{LW} \;=\; \sum_{\alpha} \hbar\omega_\alpha\, b^\dagger_\alpha b_\alpha \;+\; \tfrac{1}{3!}\sum_{\alpha,\beta,\gamma}{}' \phi_{\alpha\beta\gamma}(b^\dagger_\alpha + b_\alpha)(b^\dagger_\beta + b_\beta)(b^\dagger_\gamma + b_\gamma) \tag{1}$$

with anharmonicites $\phi_{\alpha\beta\gamma}$. Strictly, the oscillators in LW were non-linear 'russ-oscillators', as opposed to harmonic, but for the moment that's a detail (we can simply replace $\hbar\omega_\alpha b^\dagger_\alpha b_\alpha \to \epsilon_\alpha(\hat{n}_\alpha)$ with $\hat{n}_\alpha = b^\dagger_\alpha b_\alpha$).

Now consider the following model:

$$\begin{aligned} H \;=&\; \tfrac{1}{2}\epsilon\; \boldsymbol{\sigma}_z \;+\; t(\boldsymbol{\sigma}_+ + \boldsymbol{\sigma}_-) \\ &+\; \hat{1}\;\hbar\omega_0 b^\dagger_0 b_0 \\ &+ \boldsymbol{\sigma}_z \lambda(b^\dagger_0 + b_0) \\ &+\; \hat{1}\;\Big(H_{0a} \;+\; H_{LW}\Big) \end{aligned} \tag{2}$$

The first line here is a two-level system for the electron; with $\boldsymbol{\sigma}$ the Pauli matrices and the basis chosen such that the eigenstate of $\boldsymbol{\sigma}_z$ with eigenvalue $+1$ (-1) corresponds to the electron being localized in the left (right) well. Equivalently, writing $|\!\uparrow\rangle \equiv |L\rangle$ and $|\!\downarrow\rangle \equiv |R\rangle$ for an electron localized in the L or R well, we can write

$$H_{TLS} \;=\; \tfrac{1}{2}\epsilon\,\Big(|\uparrow\rangle\langle\uparrow| - |\downarrow\rangle\langle\downarrow|\Big) \;+\; t\,\Big(|\uparrow\rangle\langle\downarrow| + |\downarrow\rangle\langle\uparrow|\Big) \tag{3}$$

(in this notation the unity operator for the electron's trivial Hilbert space is $\hat{1} = (|\!\uparrow\rangle\langle\uparrow\!| + |\!\downarrow\rangle\langle\downarrow\!|)$). The quantity ϵ is of course the electronic level 'detuning', i.e. the difference in ground state energies of the electron localized in the two wells in the absence of tunneling, $t = 0$.

Let me add a comment in passing. Although we have in mind that the two-level system here corresponds to a single and, as such, non-interacting electron, this need not be the case: the TLS, and in particular the tunneling term H_t, may involve electron interactions. Negative-U centres provide an example. Consider an electronic $H_0 = \sum_{i=L,R,\sigma} \epsilon_i d^\dagger_{i\sigma} d_{i\sigma} + (U_L \hat{n}_{L\uparrow}\hat{n}_{L\downarrow} + U_R \hat{n}_{R\uparrow}\hat{n}_{R\downarrow})$, (with σ a 'real' electron spin), and with negative Hubbard $U_i < 0$. For suitable bare parameters we can focus on the two states $|L\rangle = |\!\uparrow\downarrow; -\rangle = d^\dagger_{L\uparrow} d^\dagger_{L\downarrow}|\mathrm{vac}\rangle$ and $|R\rangle = |-;\uparrow\downarrow\rangle = d^\dagger_{R\uparrow} d^\dagger_{R\downarrow}|\mathrm{vac}\rangle$ (whose energies under H_0 can be chosen as $\pm\frac{1}{2}\epsilon$ respectively, with a suitable choice of the zero of energy). These states are then coupled with a pairing interaction $H_t = t(d^\dagger_{L\uparrow} d^\dagger_{L\downarrow} d_{R\downarrow} d_{R\uparrow} + \mathrm{h.c.})$ with matrix element t. And with the basis $|L\rangle, |R\rangle$, H_t can be represented precisely as $H_t = t(|L\rangle\langle R| + |R\rangle\langle L|)$ – exactly as in eq. 3 (now with $|\!\uparrow\rangle \equiv |L\rangle$ and $|\!\downarrow\rangle \equiv |R\rangle$). The system we consider – and in particular the tunneling term – need not therefore refer exclusively to non-interacting electrons. This is conceptually important, and we return to it again in sec. V A.

The second term in eq. 2, $\hat{1}\hbar\omega_0 b^\dagger_0 b_0$, is a harmonic mode that we can view as representing a 'reaction coordinate' for electron transfer; which is linearly coupled to the electron degree of freedom in the standard way via the third term, $\boldsymbol{\sigma}_z \lambda(b^\dagger_0 + b_0) \equiv (|\!\uparrow\rangle\langle\uparrow\!| - |\!\downarrow\rangle\langle\downarrow\!|)\lambda(b^\dagger_0 + b_0)$.[1] The final term in H is the anharmonic coupling of the 0-mode to the others, H_{0a}, together with H_{LW}.

It may prove helpful to generalise the above slightly to the case where the 0-oscillator frequency depends on which well the electron is in, i.e. to replace

$$\hat{1}\;\hbar\omega_0 b^\dagger_0 b_0 \;\equiv\; \Big(|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|\Big)\hbar\omega_0 b^\dagger_0 b_0 \;\longrightarrow\; \Big(|\uparrow\rangle\langle\uparrow|\;\hbar\omega_{0\uparrow} + |\downarrow\rangle\langle\downarrow|\;\hbar\omega_{0\downarrow}\Big) b^\dagger_0 b_0. \tag{4}$$

We'll adopt this in the following, as it's readily switched off by setting $\omega_{0\uparrow} = \omega_{0\downarrow}$; likewise, we'll replace the coupling λ by λ_σ. The Hamiltonian eq. 2 can be written as follows (with $\sigma = \pm$ for $\uparrow/\downarrow$):

$$H \;=\; \sum_{\sigma} |\sigma\rangle\langle\sigma| \Big(\tfrac{\sigma}{2}\epsilon + \sigma\lambda_\sigma(b^\dagger_0 + b_0) + \hbar\omega_{0\sigma} b^\dagger_0 b_0 + \;H_{0a} \;+\; H_{LW}\Big) \;+ t\sum_{\sigma} |\sigma\rangle\langle -\sigma| \tag{5}$$

Now define

$$\tilde{b}^{\dagger}_{0\sigma} \;=\; b^{\dagger}_{0} \;+\; \sigma\frac{\lambda_{\sigma}}{\hbar\omega_{0\sigma}} \tag{6}$$

(corresponding to shifting the 0-oscillator position); s.t. $\hbar\omega_{0\sigma}b^{\dagger}_{0}b_{0} + \sigma\lambda_{\sigma}(b^{\dagger}_{0} + b_{0}) = \hbar\omega_{0\sigma}\tilde{b}^{\dagger}_{0\sigma}\tilde{b}_{0\sigma} - \lambda^{2}_{\sigma}/(\hbar\omega_{0\sigma})$ and hence

$$H \;=\; \sum_{\sigma}|\sigma\rangle\langle\sigma|\Big(\tfrac{\sigma}{2}\epsilon - \tfrac{\lambda^{2}_{\sigma}}{\hbar\omega_{0\sigma}} + \hbar\omega_{0\sigma}\tilde{b}^{\dagger}_{0\sigma}\tilde{b}_{0\sigma} + \; H_{0a} \;+\; H_{LW}\Big) \;+ t\sum_{\sigma}|\sigma\rangle\langle -\sigma| \tag{7}$$

At this stage, let's choose the anharmonic coupling H_{0a} to be

$$H_{0a} \;=\; \tfrac{1}{2}{\sum_{\beta,\gamma}}' \phi_{0\beta\gamma}(\tilde{b}^{\dagger}_{0\sigma} + \tilde{b}_{0\sigma})(b^{\dagger}_{\beta} + b_{\beta})(b^{\dagger}_{\gamma} + b_{\gamma}), \tag{8}$$

i.e. cubic – with a coupling $\phi_{0\beta\gamma}$ we've taken to be independent of $\sigma = \uparrow/\downarrow \equiv L/R$ – and of just the same form as in H_{LW}, eq. 1. By virtue of the latter we could simply include the 0-orbital in the set of orbitals contributing to H_{LW}, and thus write eq. 7 more economically as

$$H \;=\; \sum_{\sigma}|\sigma\rangle\langle\sigma|\Big(\tfrac{\sigma}{2}\epsilon - \tfrac{\lambda^{2}_{\sigma}}{\hbar\omega_{0\sigma}} \;+\; H_{LW,\sigma}\Big) \;+ t\sum_{\sigma}|\sigma\rangle\langle -\sigma| \tag{9}$$

(where the σ in $H_{LW,\sigma}$ is a reminder that the 0-orbital is σ-dependent).

The 0- and α-oscillators are of course common to both $\sigma = \uparrow$ and $\downarrow$ (albeit with the 0-oscillator shifted differently according to whether $\sigma = \uparrow/\downarrow$); so even with $t = 0$ – no electron transfer – the $|\!\uparrow\rangle \equiv |L\rangle$ and $|\!\downarrow\rangle \equiv |R\rangle$ sectors of H aren't independent. This model would enable us to assess the effect of electron tunneling on the ergodicity and many-body localization of the vibrational states, or vice versa of course.

Let's now consider another model, denoted H' and given by:

$$\begin{aligned} H' \;=\; &\sum_{\sigma}|\sigma\rangle\langle\sigma|\Big(\tfrac{\sigma}{2}\epsilon + \hbar\omega_{0\sigma}b^{\dagger}_{0\sigma}b_{0\sigma} + \tfrac{1}{2}{\sum_{\beta,\gamma}}'\phi^{(\sigma)}_{0\beta\gamma}(b^{\dagger}_{0\sigma} + b_{0\sigma})(b^{\dagger}_{\beta\sigma} + b_{\beta\sigma})(b^{\dagger}_{\gamma\sigma} + b_{\gamma\sigma}) \;+\; H^{(\sigma)}_{LW}\Big) \\ &+ t\sum_{\sigma}|\sigma\rangle\langle -\sigma| \end{aligned} \tag{10}$$

Physically, when the electron is in the $\sigma = \uparrow$ or $\downarrow$ state, it has a *distinct* set of vibrational modes to which it couples – the 0σ- and $\alpha\sigma$-modes with frequencies $\omega_{0\sigma}$ and $\omega_{\alpha\sigma}$; and with σ-dependent anharmonic couplings $\phi^{(\sigma)}_{0\beta\gamma}$ and $\phi^{(\sigma)}_{\alpha\beta\gamma}$ (for $H^{(\sigma)}_{LW} = \sum_{\alpha}\hbar\omega_{\alpha\sigma}b^{\dagger}_{\alpha\sigma}b_{\alpha\sigma} + \frac{1}{3!}{\sum}'_{\alpha,\beta,\gamma}\phi^{(\sigma)}_{\alpha\beta\gamma}(b^{\dagger}_{\alpha\sigma} + b_{\alpha\sigma})(b^{\dagger}_{\beta\sigma} + b_{\beta\sigma})(b^{\dagger}_{\gamma\sigma} + b_{\gamma\sigma}) \equiv \sum_{\alpha}\hbar\omega_{\alpha\sigma}b^{\dagger}_{\alpha\sigma}b_{\alpha\sigma} + H^{(\sigma)}_{\phi LW}$). In this case there is simply no need to have any $(b^{\dagger}_{0\sigma} + b_{0\sigma})$ coupling terms (and if they'd been there in the first place we can always eliminate them by a transformation akin to that used above). The $\phi^{(\sigma)}_{0\beta\gamma}$ couplings are again of the same form as those appearing in $H^{(\sigma)}_{LW}$ (and we've allowed the possibility that they're σ-dependent). So we can just include the 0-orbital in the set of orbitals contributing to $H^{(\sigma)}_{LW}$, to write eq. 10 more economically as

$$H' \;=\; \sum_{\sigma}|\sigma\rangle\langle\sigma|\Big(\tfrac{\sigma}{2}\epsilon \;+\; H^{(\sigma)}_{LW}\Big) \;+\; t\sum_{\sigma}|\sigma\rangle\langle -\sigma| \tag{11a}$$

$$\;=\; \sum_{\sigma}|\sigma\rangle\langle\sigma|\Big(\tfrac{\sigma}{2}\epsilon + \sum_{\alpha}\hbar\omega_{\alpha\sigma}\; b^{\dagger}_{\alpha\sigma}b_{\alpha\sigma} \;+\; H^{(\sigma)}_{\phi LW}\Big) \;+\; t\sum_{\sigma}|\sigma\rangle\langle -\sigma| \tag{11b}$$

where we've dropped explicit reference to a 0-mode (it's just one of the α-modes). This model corresponds to 'two *distinct* LW problems', coupled via the electron hopping t (and such that for $t = 0$ the $|\!\uparrow\rangle \equiv |L\rangle$ and $|\!\downarrow\rangle \equiv |R\rangle$ sectors of H' are truly independent). It could be used to consider the effect of electron tunneling on the ergodicity and many-body localization of the vibrational states; e.g. for $t = 0$, the $\sigma = \uparrow$ vibrational states of energy E might be localized, while those for $\sigma = \downarrow$ might be delocalized, and we'd like to understand what happens when the two sets of vibrational states are coupled under t.

Now consider a model, H'', specified by

$$H'' \;=\; \sum_{\sigma}|\sigma\rangle\langle\sigma|\Big(\tfrac{\sigma}{2}\epsilon \;+\; \sigma\sum_{\alpha}\lambda_{\alpha\sigma}(b^{\dagger}_{\alpha} + b_{\alpha}) \;+\; \sum_{\alpha}\hbar\omega_{\alpha\sigma}b^{\dagger}_{\alpha}b_{\alpha} \;+\; H_{an}\Big) \;+\; t\sum_{\sigma}|\sigma\rangle\langle -\sigma| \tag{12}$$

where H_{an} represents anharmonic coupling between the α-oscillators. Note that in the *absence* of H_{an}, this is a spin-boson model (see eq. 1.4 of Leggett *et al*) – which isn't exactly trivial (!). In parallel to eq. 6 above, define $\tilde{b}^{\dagger}_{\alpha\sigma} = b^{\dagger}_{\alpha} + \sigma\frac{\lambda_{\alpha\sigma}}{\hbar\omega_{\alpha\sigma}}$ such that $\hbar\omega_{\alpha\sigma}b^{\dagger}_{\alpha}b_{\alpha} + \sigma\lambda_{\sigma}(b^{\dagger}_{\alpha} + b_{\alpha}) = \hbar\omega_{\alpha\sigma}\tilde{b}^{\dagger}_{\alpha\sigma}\tilde{b}_{\alpha\sigma} - \lambda^2_{\alpha\sigma}/(\hbar\omega_{\alpha\sigma})$; whence $H'' = \sum_{\sigma}|\sigma\rangle\langle\sigma|\Big(\frac{\sigma}{2}\epsilon - \sum_{\alpha}\frac{\lambda^2_{\alpha\sigma}}{\hbar\omega_{\alpha\sigma}} + \sum_{\alpha}\hbar\omega_{\alpha\sigma}\tilde{b}^{\dagger}_{\alpha\sigma}\tilde{b}_{\alpha\sigma} + H_{an}\Big) + t\sum_{\sigma}|\sigma\rangle\langle -\sigma|$. If now we choose

$$H_{an} \;\equiv\; H^{(\sigma)}_{\phi LW} \;=\; \tfrac{1}{3!}{\sum}'_{\alpha,\beta,\gamma}\phi^{(\sigma)}_{\alpha\beta\gamma}(\tilde{b}^{\dagger}_{\alpha\sigma} + \tilde{b}_{\alpha\sigma})(\tilde{b}^{\dagger}_{\beta\sigma} + \tilde{b}_{\beta\sigma})(\tilde{b}^{\dagger}_{\gamma\sigma} + \tilde{b}_{\gamma\sigma}) \tag{13}$$

then:

$$H'' \;=\; \sum_{\sigma}|\sigma\rangle\langle\sigma|\Big(\tfrac{\sigma}{2}\epsilon \;-\; \sum_{\alpha}\frac{\lambda^2_{\alpha\sigma}}{\hbar\omega_{\alpha\sigma}} \;+\; \sum_{\alpha}\hbar\omega_{\alpha\sigma}\tilde{b}^{\dagger}_{\alpha\sigma}\tilde{b}_{\alpha\sigma} \;+\; H^{(\sigma)}_{\phi LW}\Big) \;+\; t\sum_{\sigma}|\sigma\rangle\langle -\sigma| \tag{14}$$

Two points are worth noting here:
(i) H'' is a natural extension of the first model, H, to the case where all modes are linearly coupled to $\sigma = \uparrow/\downarrow \equiv L/R$.
(ii) Modulo the $\sum_{\alpha}\lambda^2_{\alpha\sigma}/\hbar\omega_{\alpha\sigma}$ shift, H'' also formally equivalent to the H' model eq. 11; albeit that in the latter case the $b^{\dagger}_{\alpha\uparrow}$ and $b^{\dagger}_{\alpha\downarrow}$ operators are independent, while in H'' they are related by $\tilde{b}^{\dagger}_{\alpha\uparrow} = b^{\dagger}_{\alpha} + \lambda_{\alpha\uparrow}/\hbar\omega_{\alpha\uparrow}$ and $\tilde{b}^{\dagger}_{\alpha\downarrow} = b^{\dagger}_{\alpha} - \lambda_{\alpha\downarrow}/\hbar\omega_{\alpha\downarrow}$. These similarities will be seen clearly in the state-space Hamiltonians considered shortly.

II. STATE-SPACE HAMILTONIANS.

We now focus on the first model above, decomposing the Hamiltonian as:

$$\begin{aligned}
H \;&= H_0 \;+\; H_{\phi} \;+\; H_t && \text{(15a)}\\
H_0 \;&= \sum_{\sigma}|\sigma\rangle\langle\sigma|\Big(\tfrac{\sigma}{2}\epsilon - \tfrac{\lambda^2_{\sigma}}{\hbar\omega_{0\sigma}} + \hbar\omega_{0\sigma}\tilde{b}^{\dagger}_{0\sigma}\tilde{b}_{0\sigma} + \sum_{\alpha}\epsilon(\hat{n}_{\alpha})\Big) \qquad \equiv \sum_{\sigma}H_{0\sigma} && \text{(15b)}\\
H_{\phi} \;&= \sum_{\sigma}|\sigma\rangle\langle\sigma|\Big(\tfrac{1}{2}{\sum_{\beta,\gamma}}'\phi_{0\beta\gamma}(\tilde{b}^{\dagger}_{0\sigma} + \tilde{b}_{0\sigma})(b^{\dagger}_{\beta} + b_{\beta})(b^{\dagger}_{\gamma} + b_{\gamma}) \;+\; H_{\phi LW}\Big) \qquad \equiv \sum_{\sigma}H_{\phi\sigma} && \text{(15c)}\\
H_t \;&= t\sum_{\sigma}|\sigma\rangle\langle -\sigma| && \text{(15d)}
\end{aligned}$$

Note that (a) in eq. 15b we've allowed for the α-modes (of which there are N) to be non-linear russ-oscillators if we wish; and (b) $H_{\phi LW}$ in eq. 15 refers to the non-linear inter-oscillator couplings in eq. 1.

Any state of the unperturbed system can be specified by prescribing the number of quanta in each of the $N+1$ vibrational modes, together with $\sigma = \uparrow/\downarrow \equiv L/R$. The zeroth-order states of the system may thus be viewed as defining a lattice of sites, $\{i\sigma\}$, in an $(N+2)$-dimensional quantum state-space. We denote the zeroth-order site functions by $|i\sigma\rangle = |n^{(i)}_{0\sigma}; n^{(i)}_1, n^{(i)}_2 \ldots. n^{(i)}_N; \sigma\rangle \equiv |n^{(i)}_{0\sigma}; \{n^{(i)}_{\alpha}\}; \sigma\rangle$, where $n^{(i)}_{0\sigma}$ (or $n^{(i)}_{\alpha}$) labels the number of quanta in the 0σ oscillator (or α oscillator) associated with site $i\sigma$; i.e.

$$|i\sigma\rangle \;=\; |n^{(i)}_{0\sigma}; \{n^{(i)}_{\alpha}\}; \sigma\rangle \;=\; |n^{(i)}_{0\sigma}; \{n^{(i)}_{\alpha}\}\rangle \otimes |\sigma\rangle\ . \tag{16}$$

The $|i\sigma\rangle$ are eigenfunctions of H_0, so for each site there is an associated zeroth-order site energy $\epsilon_{i\sigma}$ given (eq. 15) by

$$\epsilon_{i\sigma} \;=\; \tfrac{\sigma}{2}\epsilon - \tfrac{\lambda^2_{\sigma}}{\hbar\omega_{0\sigma}} + \hbar\omega_{0\sigma}n^{(i)}_{0\sigma} + \sum_{\alpha}\epsilon(n^{(i)}_{\alpha}). \tag{17}$$

Under both the interactions embodied in H_{ϕ}, and the electron tunneling H_t, the zeroth-order sites are coupled. H can thus be represented as an effective tight-binding model in state-space, a determination of its form being the obvious first task. One slight subtlety in the problem is that the states $|n^{(i)}_{0\sigma}; \{n^{(i)}_{\alpha}\}\rangle$ (see eq. 16b) are not orthonormal for *different* σ, i.e. $\langle n^{(i)}_{0\sigma}; \{n^{(i)}_{\alpha}\}|n^{(j)}_{0-\sigma}; \{n^{(j)}_{\alpha}\}\rangle \neq \delta_{ij}$. Physically, this reflects the fact (sec. I) that the $0\uparrow$- and $0\downarrow$-oscillators are just differently displaced/shifted versions of the common underlying 0-oscillator; so the overlap between their states, $\langle n^{(i)}_{0\sigma}|n^{(j)}_{0-\sigma}\rangle$, is generally non-zero for all i, j. The construction of H is detailed in Appendix **??**, and leads to the intuitively obvious form:

$$\begin{aligned}
H \;=\; &\sum_{\sigma}\Big(\sum_{i,j}(\epsilon_{i\sigma}\delta_{ij} \;+\; V^{\sigma\sigma}_{ij})|i\sigma\rangle\langle j\sigma|\Big)\\
&+\sum_{\sigma}\Big(\sum_{i,j}t^{\sigma-\sigma}_{ij}|i\sigma\rangle\langle j-\sigma|\Big)
\end{aligned} \tag{18}$$

Here,

$$V_{ij}^{\sigma\sigma} \;=\; \langle i\sigma|H_{\phi\sigma}|j\sigma\rangle \tag{19}$$

connects state-space sites with the *same* σ under the action of the anharmonic H_ϕ (it is of course matrix elements of this type that were originally considered in LW); and we add in passing that $V_{ii}^{\sigma\sigma}=0$. By contrast, the $t_{ij}^{\sigma-\sigma}$ connect state-space sites with different σ, under the action of the electron tunneling H_t. They are given by

$$t_{ij}^{\sigma-\sigma} = t\ \langle n_{0\sigma}^{(i)};\{n_\alpha^{(i)}\}|n_{0-\sigma}^{(j)};\{n_\alpha^{(j)}\}\rangle \tag{20a}$$

$$= t\ \langle n_{0\sigma}^{(i)}|n_{0-\sigma}^{(j)}\rangle\ \prod_\alpha \delta_{n_\alpha^{(i)},n_\alpha^{(j)}} \tag{20b}$$

where the product just embodies formally the obvious fact that the hopping H_t does not change the occupation of the α-modes, so that $n_\alpha^{(i)}=n_\alpha^{(j)}$ $(\forall\alpha)$ is required; whence $t_{ij}^{\sigma-\sigma}$ is just the bare t times the overlap matrix element of the two displaced 0-modes. We also add in passing that $t_{ii}^{\sigma-\sigma}\neq 0$ (although this is not of course a strictly diagonal coupling, because $\sigma\neq-\sigma$).

A. State-space Hamiltonians H' and H''.

Now consider the second model above, H', given by eq. 11; and for which $|i\sigma\rangle=|\{n_{\alpha\sigma}^{(i)}\};\sigma\rangle$ $(=|\{n_{\alpha\sigma}^{(i)}\}\rangle\otimes|\sigma\rangle)$. The main point here is that the state-space form of H' is exactly that given in eq. 18 for H, where now: $\epsilon_{i\sigma}=\frac{\sigma}{2}\epsilon+\sum_\alpha\hbar\omega_{\alpha\sigma}n_{\alpha\sigma}^{(i)}$ from eq. 11b (cf eq. 17); $V_{ij}^{\sigma\sigma}=\langle i\sigma|H_{\phi\sigma}|j\sigma\rangle$ as in eq. 19, with $H_{\phi\sigma}=|\sigma\rangle\langle\sigma|H_{\phi LW}^{(\sigma)}=|\sigma\rangle\langle\sigma|\frac{1}{3!}\sum'_{\alpha,\beta,\gamma}\phi_{\alpha\beta\gamma}^{(\sigma)}(b_{\alpha\sigma}^\dagger+b_{\alpha\sigma})(b_{\beta\sigma}^\dagger+b_{\beta\sigma})(b_{\gamma\sigma}^\dagger+b_{\gamma\sigma})$ the anharmonicities, akin to eq. 15c; and

$$t_{ij}^{\sigma-\sigma} = t\ \langle\{n_{\alpha\sigma}^{(i)}\}|\{n_{\alpha-\sigma}^{(j)}\}\rangle \tag{21a}$$

$$= t\ \prod_\alpha\langle n_{\alpha\sigma}^{(i)}|n_{\alpha-\sigma}^{(j)}\rangle \tag{21b}$$

Next, the model H'', eq. 14. It too has precisely the state-space form given in eq. 18 for H, where now: $\epsilon_{i\sigma}=\frac{\sigma}{2}\epsilon-\sum_\alpha\lambda_{\alpha\sigma}^2/\hbar\omega_{\alpha\sigma}+\sum_\alpha\hbar\omega_{\alpha\sigma}n_{\alpha\sigma}^{(i)}$; $V_{ij}^{\sigma\sigma}=\langle i\sigma|H_{\phi\sigma}|j\sigma\rangle$ as in eq. 19, with $H_{\phi\sigma}=|\sigma\rangle\langle\sigma|H_{\phi LW}^{(\sigma)}=|\sigma\rangle\langle\sigma|\frac{1}{3!}\sum'_{\alpha,\beta,\gamma}\phi_{\alpha\beta\gamma}^{(\sigma)}(\tilde b_{\alpha\sigma}^\dagger+\tilde b_{\alpha\sigma})(\tilde b_{\beta\sigma}^\dagger+\tilde b_{\beta\sigma})(\tilde b_{\gamma\sigma}^\dagger+\tilde b_{\gamma\sigma})$ the anharmonicities (eq. 13), just as in eq. 15c; and with $t_{ij}^{\sigma-\sigma}$ again given precisely by eq. 21.

So whichever of the three models we consider, the underlying state-space Hamiltonian takes the form eq. 18. That of course shouldn't be surprising: the whole idea is to represent the Hamiltonian as an effective tight-binding model (TBM) in state-space, and eq. 18 is the most general TBM consistent with the underlying symmetries for the problems considered. But that of course means that the differences between the models – which are perfectly real – are contained in the TBM matrix elements. We do of course have a good feel, from LW and later papers, how to handle the $V_{ij}^{\sigma\sigma}$ matrix elements corresponding to the non-linear oscillator coupling (and indeed these are pretty similar for the three models considered above). A key difference between the models resides in the $t_{ij}^{\sigma-\sigma}$ elements; and as I write this I have little idea/intuition about how to handle these within an LW-like framework – what assumptions/simplifications one could/should make about the $t_{ij}^{\sigma-\sigma}$, etc. Indeed even if we neglect the anharmonicities completely, setting $V_{ij}^{\sigma\sigma}=0$, the models above remain non-trivial and are obviously controlled primarily by the $\{t_{ij}^{\sigma-\sigma}\}$. So getting some feel for how one should handle the $t_{ij}^{\sigma-\sigma}$s is obviously central. We return to this below.

III. VANISHING TUNNELING AND ANHARMONICITY: $\mathbf{H_0}$.

Focus now on the first model, specified by H. Here we consider it in the limit of zero anharmonic couplings – i.e. $H_\phi=0$ in eq. 15, so we can also forget the russ-oscillators completely – *and* of vanishing electron tunneling, $t=0$. This is as simple as it gets: in state-space language $H\equiv\sum_\sigma\sum_i\epsilon_{i\sigma}|i\sigma\rangle\langle i\sigma|$ (eq. 18), so the states are completely localized in the Fock space of shifted oscillator states. But there are still issues to think through.

The Hamiltonian we consider here is then

$$H_0 \;=\; \sum_\sigma |\sigma\rangle\langle\sigma|\Big(\tfrac{\sigma}{2}\epsilon + \sigma\lambda_\sigma(b_0^\dagger + b_0) + \hbar\omega_{0\sigma} b_0^\dagger b_0\Big) \qquad \equiv \sum_\sigma H_{0\sigma} \tag{22a}$$

$$\;=\; \sum_\sigma |\sigma\rangle\langle\sigma|\Big(\tfrac{\sigma}{2}\epsilon - \tfrac{\lambda_\sigma^2}{\hbar\omega_{0\sigma}} + \hbar\omega_{0\sigma}\tilde{b}_{0\sigma}^\dagger \tilde{b}_{0\sigma}\Big) \tag{22b}$$

– separable into disjoint $\uparrow \equiv L$ and $\downarrow \equiv R$ sectors, each corresponding to a different shift of the common 0-oscillator.

First recall (see Appendix **??**) that the normalized eigenfunctions, $|\alpha, n\rangle$, and eigenvalues for a single shifted oscillator

$$\tilde{H}_s \;=\; (b^\dagger - \alpha)(b - \alpha) \;=\; b^\dagger b \;-\; \alpha(b^\dagger + b) + \alpha^2 \tag{23}$$

are given by

$$|\alpha, n\rangle \;=\; D(\alpha)|n\rangle \qquad \tilde{H}_s|\alpha, n\rangle \;=\; n\;|\alpha, n\rangle \tag{24}$$

in terms of the usual SHO states $|n\rangle$ of the unshifted oscillator; with a displacement operator[2]

$$D(\alpha) \;=\; e^{\alpha(b^\dagger - b)} \qquad :\; D(\alpha)D^\dagger(\alpha) \;=\; 1 \tag{25}$$

satisfying (eq. **??**)

$$bD(\alpha) \;= D(\alpha)(b + \alpha) \tag{26a}$$

$$b^\dagger D(\alpha) \;= D(\alpha)(b^\dagger + \alpha) \tag{26b}$$

(and $\langle\alpha, n|\alpha, n\rangle = 1$ by the unitarity of $D(\alpha)$). Hence

$$|\alpha, n+1\rangle \;=\; D(\alpha)|n+1\rangle \;=\tfrac{1}{\sqrt{n+1}}D(\alpha)b^\dagger|n\rangle \tag{27a}$$

$$\;=\tfrac{1}{\sqrt{n+1}}(b^\dagger - \alpha)|\alpha, n\rangle \tag{27b}$$

(from eq. 26b); i.e. $|\alpha, n+1\rangle = \frac{1}{\sqrt{n+1}}(b^\dagger - \alpha)|\alpha, n\rangle$, so the $|\alpha, n\rangle$ can be generated from the ground state $|\alpha, 0\rangle$ by repeated application of $(b^\dagger - \alpha)$, *viz*

$$|\alpha, n\rangle \;=\; \frac{1}{\sqrt{n!}}(b^\dagger - \alpha)^n|\alpha, 0\rangle\;. \tag{28}$$

Let's then look at the g.s. $|\alpha, 0\rangle$. To that end recall BCH (=Baker-Campbell-Hausdorff equality), *viz*

$$\exp(\hat{X})\exp(\hat{Y}) \;=\; \exp\Big(\hat{X} + \hat{Y} + \tfrac{1}{2}[\hat{X}, \hat{Y}]\Big) \tag{29}$$

provided $\hat{X}$ and $\hat{Y}$ each commute with $[\hat{X}, \hat{Y}]$ (in our case $\hat{X}$, $\hat{Y}$ will be either of b, $b^\dagger$, and $[b, b^\dagger] = 1$, so this condition is satisfied). This gives $e^{\alpha b^\dagger}e^{-\alpha b} = e^{\alpha(b - b^\dagger)}e^{\frac{1}{2}\alpha^2} = D(\alpha)e^{\frac{1}{2}\alpha^2}$, i.e.

$$D(\alpha) \;\equiv\; e^{-\frac{1}{2}\alpha^2}e^{\alpha b^\dagger}e^{-\alpha b} \tag{30}$$

(so $D(\alpha) = e^{\alpha(b^\dagger - b)}$ and $e^{\alpha b^\dagger}e^{-\alpha b}$ are equivalent modulo a constant). Hence

$$|\alpha, 0\rangle \;=\; D(\alpha)|0\rangle \;= e^{-\frac{1}{2}\alpha^2}e^{\alpha b^\dagger}e^{-\alpha b}|0\rangle \tag{31a}$$

$$\;= e^{-\frac{1}{2}\alpha^2}e^{\alpha b^\dagger}|0\rangle \tag{31b}$$

where eq. 31b arises because $b|0\rangle = 0$ [and by the same token the g.s. is a coherent state, i.e. is an eigenfunction of b: $bD(\alpha)|0\rangle = D(\alpha)(b+\alpha)|0\rangle$ (eq. 26a), whence $bD(\alpha)|0\rangle = \alpha\,|0\rangle$]. Since $b^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$ we have $(b^\dagger)^n|0\rangle = \sqrt{n!}|0\rangle$, $\implies\; e^{\alpha b^\dagger}|0\rangle = \sum_{n=0}^\infty \frac{\alpha^n}{n!}(b^\dagger)^n|0\rangle = \sum_{n=0}^\infty \frac{\alpha^n}{\sqrt{n!}}|n\rangle$ and hence the ground state

$$|\alpha, 0\rangle \;=\; e^{-\frac{1}{2}\alpha^2}\sum_{n=0}^\infty \frac{\alpha^n}{\sqrt{n!}}\;|n\rangle\;. \tag{32}$$

Since $|\alpha,0\rangle$ is a shifted oscillator state, it is (by definition) completely localized in the Fock space of shifted oscillator states. But we can of course ask about its localization characteristics in the state-space $\{|m\rangle\}$ of the 'original' unshifted oscillator states. This is embodied in the inverse participation ratio (IPR), defined just as for localization in real-space: if $|\Phi_\alpha\rangle$ is a normalized real-space wavefunction (of energy E_α) expressed as a linear combination of orthonormal real-space site wavefunctions $\{|m\rangle\}$, i.e. $|\Phi_\alpha\rangle = \sum_m a_{m\alpha}|m\rangle$ with $a_{m\alpha} = \langle m|\Phi_\alpha\rangle$, then the IPR $L(E_\alpha)$ is given by $L(E_\alpha) = \sum_m |a_{m\alpha}|^4$. If the state is localized then $L(E_\alpha)$ is non-zero ($L(E_\alpha) \sim 1/n_s$ for a state uniformly spread over n_s sites); while for a delocalized/extended state the IPR vanishes. In our present context,

$$P_m \;:=\; |a_{m\alpha}|^2 \;=\; |\langle m|\alpha,0\rangle|^2 \;=\; e^{-\alpha^2}\frac{\alpha^{2m}}{m!} \qquad : \text{ m} = 0,1,2,... \tag{33}$$

This is a Poisson distribution for discrete $m = 0,1,2...$, of standard form $P_m(\lambda) = (\lambda^m/m!)e^{-\lambda}$ with parameter $\lambda = \alpha^2$ [for which the both the mean and variance equal λ, i.e. $\langle m\rangle = \sum_m mP_m = \lambda$, $\mathrm{Var}(m) = \langle(m-\langle m\rangle)^2\rangle = \lambda$, and hence $\langle m^2\rangle = \lambda(\lambda+1)$]. What we require here is clearly

$$L(E_\alpha) \;=\; \sum_{m=0}^{\infty} P_m^2 \;=\; e^{-2\alpha^2}\sum_{m=0}^{\infty}\frac{\alpha^{4m}}{(m!)^2} \;=\; e^{-2\alpha^2}I_0(2\alpha^2) \tag{34}$$

(with $E_\alpha = 0$ for all values of the shift parameter α, since we're considering the g.s. with $n = 0$ (see eq. 24)). From GR pg 961, §8.447:1, $\sum_{k=0}^{\infty} z^{2k}/(k!)^2 = I_0(2z)$ with $I_0(z)$ a modified Bessel function of the first kind;[3] whence $L(E_\alpha) = e^{-2\alpha^2}I_0(2\alpha^2)$ ($\equiv e^{-x}I_0(x)$ with $x = 2\alpha^2$). From Abramowitz and Stegun (A&S) pg 375, §9.6.12 and pg 377, §9.7.1, we have the following asymptotics

$$I_0(z) \overset{z\to 0}{\sim} 1 + \frac{\frac{1}{4}z^2}{(1!)^2} + \frac{(\frac{1}{4}z^2)^2}{(2!)^2} + ... \qquad I_0(z) \overset{z\to\infty}{\sim} \frac{e^z}{\sqrt{2\pi z}}\left(1 + \frac{1}{8z} + \frac{3^2}{2!(8z)^2} + \frac{3^2\times 5^2}{3!(8z)^3} + ...\right)$$

(of which the former is trivially obvious from eq. 34 and the latter holds for $|\arg(z)| < \frac{1}{2}\pi$ as applicable in our case). Hence,

$$L(E_\alpha) \overset{|\alpha|\to 0}{\sim} 1 \qquad L(E_\alpha) \overset{|\alpha|\to\infty}{\sim} \frac{1}{2\sqrt{\pi}\alpha}\left(1 + \frac{1}{16\alpha^2} + \mathcal{O}(\alpha^{-4})\right), \tag{35}$$

and we note that $e^{-x}I_0(x)$ is shown in Fig 9.8 (pg 375) of A&S, and indeed decays monotonically with increasing x from its value of unity for $x = 0$.

The bottom line here is clear: for all finite α the IPR for the ground state wavefunction is thus non-zero; which means that states are also localized in the original oscillator basis $\{|m\rangle\}$ for any finite linear coupling embodied in the parameter α; and indeed even for large α are spread over only $\sim \alpha$ sites in 'original-oscillator state-space' (see eq. 35). We have of course considered explicitly the IPR only for the ground state $|\alpha,0\rangle$ (a coherent-state), but these qualitative conclusions will certainly hold for general states $|\alpha,n\rangle$.[4] To handle general states $|\alpha,n\rangle$ it is in fact helpful to generalise everything above to the case where the shift parameter α is complex, and then take α pure real at the end of the day. As discussed in the aside cc'd out in the tex file here, this enables a general result to be obtained for the probability $P_m = |\langle m|\alpha,n\rangle|^2$ for arbitrary states $|\alpha,n\rangle$ (cf eq. 33 for the ground state).

Before proceeding, let's digress briefly to comment on

$$H_0'' \;=\; \sum_\sigma |\sigma\rangle\langle\sigma|\Big(\tfrac{\sigma}{2}\epsilon \;+\; \sigma\sum_\alpha \lambda_{\alpha\sigma}(b_\alpha^\dagger + b_\alpha) \;+\; \sum_\alpha \hbar\omega_{\alpha\sigma}b_\alpha^\dagger b_\alpha\Big) \qquad \equiv \sum_\sigma H_{0\sigma}'' \tag{36a}$$

$$\;=\; \sum_\sigma |\sigma\rangle\langle\sigma|\Big(\tfrac{\sigma}{2}\epsilon \;-\; \sum_\alpha \frac{\lambda_{\alpha\sigma}^2}{\hbar\omega_{\alpha\sigma}} \;+\; \sum_\alpha \hbar\omega_{\alpha\sigma}\tilde{b}_{\alpha\sigma}^\dagger\tilde{b}_{\alpha\sigma}\Big) \tag{36b}$$

(cf eq. 22), with shifted oscillator $\tilde{b}_{\alpha\sigma} = b_\alpha + \sigma\frac{\lambda_{\alpha\sigma}}{\hbar\omega_{\alpha\sigma}}$ as usual. This is the zeroth-order limit of the model H'' (eq. 12) considered in sec. I, and $H_0'' + H_t$ is of course a spin-boson model. Once again – just as for H_0 considered above – in state-space language $H_0'' \equiv \sum_\sigma\sum_i \epsilon_{i\sigma}|i\sigma\rangle\langle i\sigma|$ (eq. 18): the states are completely localized in the Fock space of shifted oscillator states. Although the spin-boson model has many oscillators $\{\alpha\}$, they are each *harmonic* and coupled only *linearly*; and the above Fock space localization for $t = 0$ is the quantum analogue of the clasically regular/non-ergodic behaviour of such a system. If by contrast non-linear couplings of e.g. the LW variety are included in the problem, then quantum ergodicity – and relatedly (but not synonymously) delocalization in state/Fock-space – may arise even for $t = 0$. This of course we know perfectly well (!). But the point here is I think worth making, to emphasize a key difference between the models we're interested in and spin-boson models.

Digression over – now back again to H_0.

A. States of H_0, and tunnel couplings

The Hamiltonian $H_0 = \sum_\sigma H_{0\sigma}$ (eq. 22) is separable, with a dimensionless shift parameter α_σ that is σ-dependent and given (on comparison of eq. 22 to eqs. 23,24) by

$$\alpha_\sigma \;=\; -\,\sigma\frac{\lambda_\sigma}{\hbar\omega_{0\sigma}} \tag{37}$$

(with $\sigma = \pm$ for $\uparrow/\downarrow$ as usual). The eigenfunctions of $H_{0\sigma}$ are clearly

$$|\alpha_\sigma, n\rangle \otimes |\sigma\rangle \;=\; D(\alpha_\sigma)|n\rangle \otimes |\sigma\rangle \;, \tag{38}$$

with eigenvalues $\epsilon_{n\sigma} \equiv \epsilon_\sigma(n)$ given (from eqs. 23,24 and eq. 22) by

$$\epsilon_{n\sigma} \;=\; \tfrac{\sigma}{2}\epsilon \;+\; [n - \alpha_\sigma^2]\hbar\omega_{0\sigma} \;=\; \tfrac{\sigma}{2}\epsilon \;-\; \frac{\lambda_\sigma^2}{\hbar\omega_{0\sigma}} \;+\; n\,\hbar\omega_{0\sigma} \tag{39}$$

(this of course is equivalently just the site-energy $\epsilon_{i\sigma}$ of eq. 17). Note that $\frac{\lambda_\sigma^2}{\hbar\omega_{0\sigma}}$ is often referred to as the 'reorganisation energy'; for physically obvious reasons, as it gives the reduction in the oscillator energy levels relative to the uncoupled limit $\lambda_\sigma = 0$.

Under $H_t = t\sum_\sigma |\sigma\rangle\langle -\sigma|$, the tunnel matrix element between states $\langle\downarrow|\langle\alpha_\downarrow, m|$ and $|\alpha_\uparrow, n\rangle|\uparrow\rangle$ is

$$t_{m\downarrow;n\uparrow} \;=\; t\langle\alpha_\downarrow, m|\alpha_\uparrow, n\rangle \;=\; tS_{m\downarrow;n\uparrow} \tag{40}$$

(as in eq. 20 for $t_{ij}^{\sigma-\sigma} \equiv t_{i\sigma;j-\sigma}$, there for the full H); with

$$S_{m\downarrow;n\uparrow} \;=\; \langle\alpha_\downarrow, m|\alpha_\uparrow, n\rangle \;=\; \langle m|D^\dagger(\alpha_\downarrow)D(\alpha_\uparrow)|n\rangle \tag{41}$$

the overlap matrix element – or Franck-Condon factor – reflecting the non-orthogonality of the shifted oscillator states for different σ, such that

$$S_{m\downarrow;n\uparrow} \;=\; S_{n\uparrow;m\downarrow} \tag{42}$$

from reality of the wavefunctions. $S_{m\downarrow;n\uparrow}$ is considered in detail in Appendix **??**. For the completely general case, i.e. σ-distinct $\omega_{0\sigma}$ and λ_σ, the overlap $S_{m\downarrow;n\uparrow}$ is given in integral form by eq. **??**. For the case where $\lambda_\uparrow \neq \lambda_\downarrow$ is allowed but the $\uparrow$- and $\downarrow$-oscillator frequencies coincide ($\omega_{0\sigma} \equiv \omega_0$) – which is clearly the most obvious/natural one to consider – $S_{m\downarrow;n\uparrow}$ is given explicitly by eqs. **??**,**??** in terms of exponentials and associated Laguerre polynomials; and satisfies $S_{m\downarrow;n\uparrow} = \;(-1)^{m-n}S_{n\downarrow;m\uparrow}$ (eq. **??**).

Our aim now is to obtain some understanding of the issue raised at the end of sec. II A: what are the dominant matrix elements $t_{m\sigma;n-\sigma}$ which, under the electron tunneling H_t, connect the $\sigma = \uparrow/\downarrow$ shifted oscillators? To this end (for reasons given below) we first consider the position of the crossing point between the two shifted-oscillator potential energy curves, and hence the quantum number for each oscillator to which the crossing point corresponds (to the nearest integer, obviously). This is detailed in Appendix **??**, in particular sec. **??**. Note that from now on we *consider explicitly the case where the frequencies of the* $\uparrow$*- and* $\downarrow$*-oscillators are the same*, $\omega_{0\uparrow} = \omega_{0\downarrow} \equiv \omega_0$; but allow for the couplings $\lambda_\uparrow \neq \lambda_\downarrow$ if we choose.

The real-space position of the minimum in the shifted oscillator σ is denoted $x_{0\sigma}$, and its dimensionless equivalent by $\bar{x}_{0\sigma} := x_{0\sigma}/l$ where l is the natural length scale for an oscillator of frequency ω_0 and mass m, *viz* (eq. **??**) $l = \sqrt{\hbar/m\omega_0}$ ($\equiv \sqrt{\hbar\omega_0/k}$ with k the force constant). $\bar{x}_{0\sigma}$ is given by (eq. **??**)

$$\bar{x}_{0\sigma} \;=\; -\,\sigma\frac{\sqrt{2}\lambda_\sigma}{\hbar\omega_0} \;=\; \sqrt{2}\alpha_\sigma \tag{43}$$

(such that $\bar{x}_{0\uparrow} < 0$ and $\bar{x}_{0\downarrow} > 0$, consistent with the terminology $\uparrow \equiv L$ and $\downarrow \equiv R$); and the separation between the $\uparrow$- and $\downarrow$-oscillator minima, $\delta\bar{x} = \delta x/l$, follows as

$$\delta\bar{x} \;=\; \bar{x}_{0\uparrow} \;-\; \bar{x}_{0\downarrow} \;=-\frac{\sqrt{2}(\lambda_\uparrow + \lambda_\downarrow)}{\hbar\omega_0} \qquad (\equiv \sqrt{2}(\alpha_\uparrow - \alpha_\downarrow)) \;. \tag{44}$$

The crossing point $\bar{x}_{cp}$ between the potential curves is obtained in Appendix **??** (eq. **??**), from which follow the quantum numbers corresponding to the oscillator levels closest to the crossing point; *viz* (eq. **??**)

$$\downarrow-\text{oscillator}: \quad m \;=\; \tfrac{1}{4}\left[\frac{\epsilon}{(\lambda_\uparrow+\lambda_\downarrow)} \;+\; \frac{2\lambda_\downarrow}{\hbar\omega_0}\right]^2 ; \qquad \uparrow-\text{oscillator}: \quad n \;=\; \tfrac{1}{4}\left[\frac{\epsilon}{(\lambda_\uparrow+\lambda_\downarrow)} \;-\; \frac{2\lambda_\uparrow}{\hbar\omega_0}\right]^2 \tag{45}$$

such that

$$m \;-\; n \;=\; \frac{\epsilon}{\hbar\omega_0} \;-\; \frac{[\lambda_\uparrow^2-\lambda_\downarrow^2]}{(\hbar\omega_0)^2} \qquad (\equiv\; \epsilon_{m\downarrow}=\epsilon_{n\uparrow}) \tag{46}$$

(and of course $\epsilon_{m\downarrow}=\epsilon_{n\uparrow}$ – see eq. 39, which gives eq. 46 directly).

To think about this pictorially, consider the case $\lambda_\uparrow=\lambda_\downarrow\equiv\lambda$ (for which we note that $m\geq n$ for any $\epsilon\geq 0$ – as is physically obvious). Here, m and n are given by

$$m \;=\; \left[\frac{\epsilon}{4\lambda}+\frac{\lambda}{\hbar\omega_0}\right]^2, \qquad n \;=\; \left[\frac{\epsilon}{4\lambda}-\frac{\lambda}{\hbar\omega_0}\right]^2 \tag{47}$$

– i.e. two parabolae in $\epsilon/4\lambda$, symmetrically disposed about $\epsilon=0$ and centred on $\epsilon/4\lambda=+\lambda/\hbar\omega_0$ for n and on $-\lambda/\hbar\omega_0$ for m. The parabolae intersect at $\epsilon=0$, for which $m=n=(\lambda/\hbar\omega_0)^2$ ($\sim$ the ratio of the reorganisation energy to $\hbar\omega_0$). On increasing $\epsilon/4\lambda$ from 0, m continually increases, while n initially decreases until $\epsilon/4\lambda=\lambda/\hbar\omega_0$ where $n=0$ (the minimum of the n-parabola); while for $\epsilon\gg 4\lambda^2/\hbar\omega_0$ ($\sim$ the reorganisation energy), we have $m\sim(\epsilon/4\lambda)^2\sim n$ to leading order, but with a difference $m-n=\epsilon/\hbar\omega_0$ which progressively grows with increasing ϵ. Notice further that the condition eq. **??** for the 'Marcus inverted regime' is $\frac{\epsilon}{4\lambda}>\frac{\lambda}{\hbar\omega_0}$ – which thus sets in at the minimum of the n-parabola.

Now let's consider the 'strong coupling' regime, defined formally by[5]

$$\frac{\lambda_\uparrow^2+\lambda_\downarrow^2}{\hbar\omega_0} \;\gg\; \hbar\omega_0 \qquad \text{or} \qquad |\delta\bar{x}| \;\gg\; 1 \;\Longrightarrow\; \lambda_\uparrow+\lambda_\downarrow \;\gg\; \hbar\omega_0 \tag{48}$$

(the latter using eq. 44 for $\delta\bar{x}$). The two definitions are in essence equivalent (and each requires that at least one of the $\lambda_\sigma\gg\hbar\omega_0$). In physical terms, the first states that the total reorganisation energy should exceed the level-spacing $\hbar\omega_0$; while the second is that the separation between the minima of the two potential energy curves should be large (compared to the natural length l). Given the latter in particular, it is physically obvious that in the strong coupling regime the electron tunneling matrix elements $t_{m\downarrow;n\uparrow}=tS_{m\downarrow;n\uparrow}$ (eq. 40) are small, as the overlap $S_{m\downarrow;n\uparrow}$ will be strongly suppressed – as clear directly from eqs. **??**,**??**, which give $S_{m\downarrow;n\uparrow}\propto\sqrt{n!/m!}\exp(-\frac{1}{4}[\delta\bar{x}]^2)|\delta\bar{x}|^{(m-n)}$ (for $m\geq n$, and ignoring the associated Laguerre's).

I take it as more or less obvious that the physics is dominated by levels in the vicinity of the crossing point, in which sense the dominant $t_{m\sigma;n-\sigma}$ are those connecting such states. As pointed out by Onucic and PGW for example (J. Phys. Chem. **92**, 6495 (1988), referred to as 'OW'), the electron transfer rate for $kT\gg\hbar\omega_0$ is clearly dominated by levels near the crossing region.

So let's think through some initial implications of this (however obvious some are!), considering as such the Hamiltonian H_0+H_t. The local propagator for any level/site $l\sigma$ is denoted for brevity by $G_{l\sigma}(E)$ ($\equiv G_{l\sigma;l\sigma}(E)$). The retarded $G_{m\downarrow}(E)$ is given quite generally by

$$G_{m\downarrow}(E) \;=\; \Big[E \;+\; i\eta \;-\; \epsilon_{m\downarrow} \;-\; S_{m\downarrow}(E)\Big]^{-1} \tag{49}$$

(where $\eta=0+$); with $S_{m\downarrow}(E)=E_{m\downarrow}(E)-i\Delta_{m\downarrow}(E)$ the usual Feenberg self-energy, under the hopping H_t. Consider first the case where only two levels $m\!\downarrow$ and $n\!\uparrow$ in the vicinity of the crossing point are considered as being coupled under $t_{m\downarrow;n\uparrow}$. Since a pair of connected levels amounts trivially to a one-stage Cayley tree, the self-energy reduces to

$$S_{m\downarrow}(E) \;=\; t^2_{m\downarrow;n\uparrow}G^{(m\downarrow)}_{n\uparrow}(E)\;; \tag{50}$$

where (as usual) $G^{(m\downarrow)}_{n\uparrow}(E)$ is the local propagator for level/site $n\!\uparrow$, but with site $m\!\downarrow$ removed, here given by $1/(E+i\eta-\epsilon_{n\uparrow})$. Hence in this simple case eq. 49 becomes

$$G_{m\downarrow}(E) \;=\; \left[E \;+\; i\eta \;-\; \epsilon_{m\downarrow} \;-\; \frac{t^2_{m\downarrow;n\uparrow}}{(E+i\eta-\epsilon_{n\uparrow})}\right]^{-1}. \tag{51}$$

This of course is familiar and trivial – it's the local propagator for a simple two-level system, where the poles of the propagator give the (usual 'bonding/antibonding') eigenvalues, *viz* $E_{\pm} = \frac{1}{2}(\epsilon_{m\downarrow} + \epsilon_{n\uparrow}) \pm \sqrt{[\frac{1}{2}(\epsilon_{m\downarrow} - \epsilon_{n\uparrow})]^2 + t^2_{m\downarrow;n\uparrow}}$. Denoting $|l\sigma\rangle = |\alpha_\sigma, l\rangle \otimes |\sigma\rangle$, the normalized eigenfunctions $|\Psi_\beta\rangle$ for a state of energy E_β are given quite generally by

$$|\Psi_\beta\rangle \;=\; \sum_{l,\sigma} a_{l\sigma;\beta}|l\sigma\rangle \tag{52}$$

with corresponding IPR

$$L(E_\beta) \;=\; \sum_{l,\sigma} |a_{l\sigma;\beta}|^4 \;; \tag{53}$$

and thus in the present case $|\Psi_\pm\rangle = a_{m\downarrow;\pm}|m\downarrow\rangle + a_{n\uparrow;\pm}|n\uparrow\rangle$, with the $|a_{m\downarrow;\pm}|^2$ given by the residues of the poles of $G_{m\downarrow}(E)$ at $E = E_\pm$. In the particular case where $\epsilon_{m\downarrow} = \epsilon_{n\uparrow}$ — as it is at the crossing point (modulo detuning due to eqs. 45 holding only to the nearest integer) — then $E_\pm = \epsilon_{m\downarrow} \pm |t_{m\downarrow;n\uparrow}|$, and $|a_{m\downarrow;\pm}|^2 = \frac{1}{2} = |a_{n\uparrow;\pm}|^2$ such that $L(E_\pm) = \frac{1}{2}$ for both states (i.e. the degenerate states $|m\downarrow\rangle$ and $|n\uparrow\rangle$ participate equally in each of the two states).

The most obvious and important fact above is of course that the resultant states are localized (only two states are involved!), as reflected in the fact that the imaginary part of the self-energy $\Delta_{l\sigma}(E) = -\mathrm{Im}S_{l\sigma}(E)$ at $E = E_\beta$ is itself proportional to $\eta = 0+$ and hence vanishingly small; according quite generally to (see e.g. LW eq. (12))

$$\frac{\Delta_{l\sigma}(E_\beta)}{\eta} \;=\; \frac{1}{|a_{l\sigma;\beta}|^2} \;-\; 1 \qquad\qquad \Longrightarrow \quad L(E_\beta) \;=\; \sum_{l,\sigma}\left[1 + \frac{\Delta_{l\sigma}(E_\beta)}{\eta}\right]^{-2} \tag{54}$$

such that the IPR is non-vanishing (in the present example $\Delta_{m\downarrow}(E)/\eta = t^2_{m\downarrow;n\uparrow}/[(E - \epsilon_{m\downarrow})^2 + \eta^2]$ so that, for $\epsilon_{m\downarrow} = \epsilon_{n\uparrow}$ where $E_\pm = \epsilon_{m\downarrow} \pm |t_{m\downarrow;n\uparrow}|$, we have $\Delta_{m\downarrow}(E_\pm)/\eta = 1$ $[= \Delta_{n\uparrow}(E_\pm)/\eta]$ and hence $L(E_\pm) = \frac{1}{2}$ as above).

More to be put in here, will fill in later, but ....

IV. A WORKING THEORY: BASIC EQUATIONS

Let me just dive in, as I think I now see how to proceed.

We consider the full Hamiltonian $H = H_0 + H_\phi + H_t$ (eq. 15); and will also allow the anharmonic couplings to be σ-dependent, $\phi_{0\beta\gamma} \equiv \phi^{(\sigma)}_{0\beta\gamma}$ and $\phi_{\alpha\beta\gamma} \equiv \phi^{(\sigma)}_{\alpha\beta\gamma}$. We'll also have in mind the most relevant case discussed above, of common oscillator frequencies $\omega_{0\uparrow} = \omega_{0\downarrow} \equiv \omega_0$ (but $\lambda_\uparrow \neq \lambda_\downarrow$ if we wish), and the strong coupling regime $[\lambda^2_\uparrow + \lambda^2_\downarrow]^{1/2} \gg \hbar\omega_0$ (eq. 48); albeit that neither is I think strictly necessary in the following.

The state-space language of sec. II will be used, and we'll be considering the state-space Hamiltonian in its general tight-binding form eq. 18. In the following I take as given the discussion of §III in LW, which will be referred to from time to time; it will be useful in particular to refer to fig. 1 therein.

Considering the site-diagonal propagator for state-space site $j\sigma$,

$$G_{j\sigma}(E) \;=\; \left[E^+ - \epsilon_{j\sigma} - S_{j\sigma}(E)\right]^{-1} \tag{55}$$

(with $E^+ = E + i\eta$), we approximate the full *renormalized* perturbation series (RPS) for the self-energy $S_{j\sigma}(E)$ as

$$S_{j\sigma}(E) \simeq \sum_l{}' |V_{jl}^{\sigma\sigma}|^2 G_{l\sigma}(E) + \sum_k |t_{jk}^{\sigma-\sigma}|^2 G_{k-\sigma}(E) \tag{56a}$$

$$= \sum_l{}' \frac{|V_{jl}^{\sigma\sigma}|^2}{E^+ - \epsilon_{l\sigma} - S_{l\sigma}(E)} + \sum_k \frac{|t_{jk}^{\sigma-\sigma}|^2}{E^+ - \epsilon_{k-\sigma} - S_{k-\sigma}(E)} . \tag{56b}$$

(the prime denotes $l \neq j$ in the sum). Here (as in fig. 1 of LW), those sites connected to site j (strictly $j\sigma$) under the anharmonic interactions, and thus in the *same* σ-sector of state-space, are denoted as l (strictly $l\sigma$); by contrast, those connected to j under the electron tunnel coupling, and thus in the opposite sector ($-\sigma$), are denoted as sites k.

Some comments.[6] First, granted that (as in LW) the $V_{jl}^{\sigma\sigma}$ couplings arising from H_ϕ have the topology of a Bethe lattice (BL, with connectivity K), the $\mathcal{O}(V^2)$ term in eq. 56 is all that survives for $t_{jk}^{\sigma-\sigma} = 0$ (i.e. there are no higher-order terms in V in the RPS). For $t_{jk}^{\sigma-\sigma} \neq 0$, eq. 56 holds to leading (second) order in the $t_{jk}^{\sigma-\sigma}$ and $V_{jl}^{\sigma\sigma}$, which should certainly be adequate at least in strong coupling where the $t_{jk}^{\sigma-\sigma}$ tunnel couplings are small (sec. III A).[7]

Second, it is worth noting parenthetically that eq. 56 includes multiple recrossings (to arbitrary order) between the σ- and -σ-sectors of state-space, i.e. multiple recrossings of the barrier. To see this, separate eq. 56 in obvious notation as $S_{j\sigma} = S_{j\sigma}^{(v)} + S_{j\sigma}^{(t)}$ (dropping the E-dependence for clarity), and define $g_{j\sigma}^{(v)} = [E^+ - \epsilon_{j\sigma} - S_{j\sigma}^{(v)}]^{-1}$. Then eq. 55 becomes $G_{j\sigma} = g_{j\sigma}^{(v)}/[1 - g_{j\sigma}^{(v)} S_{j\sigma}^{(t)}]$, iteration of which gives

$$G_{j\sigma} = g_{j\sigma}^{(v)} + g_{j\sigma}^{(v)} S_{j\sigma}^{(t)} g_{j\sigma}^{(v)} + g_{j\sigma}^{(v)} S_{j\sigma}^{(t)} g_{j\sigma}^{(v)} S_{j\sigma}^{(t)} g_{j\sigma}^{(v)} + \ldots \tag{57}$$

Truncation of the series at the first term here corresponds to setting $t_{jk}^{\sigma-\sigma} = 0$ – an initially prepared excitation thus remains forever in the σ-sector of state-space. The second term corresponds to one crossing from the σ- to the -σ-sector (and back again, remembering that $G_{j\sigma}$ is the local/diagonal propagator). And the third and higher terms obviously correspond to multiple recrossings from the σ- to -σ-sectors.

Third, as in LW, the $V_{jl}^{\sigma\sigma}$ couplings are treated as independent random variables; with a probability distribution denoted by $g_\sigma(V_{jl}^{\sigma\sigma})$, which may be σ-dependent (reflecting different anharmonic couplings in the $\sigma = \uparrow \equiv L$ or $\downarrow \equiv R$ sectors). Likewise as detailed in LW (§III), for any site l connected under $V_{jl}^{\sigma\sigma}$ to site j, we write

$$\epsilon_{l\sigma} = \epsilon_{j\sigma} + \xi_{l\sigma} \tag{58}$$

with $\xi_{l\sigma}$ distributed essentially symmetrically about $\xi_{l\sigma} = 0$. We denote its distribution by $P_\sigma(\xi_{l\sigma})$, allowing formally for it to depend on σ (although any such effect is likely to be very small in the case where $\omega_\sigma = \omega_0$ for either σ).

Now turn to the $|t_{jk}^{\sigma-\sigma}|^2$ terms in eq. 56. Recall (eq. 20)

$$t_{jk}^{\sigma-\sigma} = t\, \langle n_{0\sigma}^{(j)}; \{n_\alpha^{(j)}\} | n_{0-\sigma}^{(k)}; \{n_\alpha^{(k)}\}\rangle = t\, \langle n_{0\sigma}^{(j)} | n_{0-\sigma}^{(k)}\rangle \prod_\alpha \delta_{n_\alpha^{(j)}, n_\alpha^{(k)}} = t\, S_{j\sigma;k-\sigma} \prod_\alpha \delta_{n_\alpha^{(j)}, n_\alpha^{(k)}} \tag{59}$$

i.e. the quantum numbers of the α-oscillators remain the same under H_t. The topology of the underlying state-space can then be viewed in terms of two 'parallel BLs': two BLs – one for $\sigma = \uparrow$ and one for $\sigma = \downarrow$ – parallel to either other, and with one displaced vertically relative to the other; such that a $\sigma = \uparrow$ state-space site $|j\uparrow\rangle = |n_{0\uparrow}^{(j)} = n_{0j}; \{n_\alpha^{(j)}\}; \uparrow\rangle$ lies directly above (or below!) the $\sigma = \downarrow$ state-space site $|j\downarrow\rangle = |n_{0\downarrow}^{(j)} = n_{0j}; \{n_\alpha^{(j)}\}; \downarrow\rangle$ (with the same number of quanta in its shifted 0-oscillator and the same $\{n_\alpha^{(j)}\}$).

A given site $j\sigma$ will be connected to a *range* of sites k-σ in which the α-oscillator quantum numbers are common to both (eq. 59). As such, the topology of the overall state-space is not strictly that of a BL; but is in practice rendered so by use of the leading-order RPS result for $S_{j\sigma}(E)$ (eq. 56). We denote by K_t the number of sites in the -σ-BL to which a given site in the σ-BL is coupled under $t_{jk}^{\sigma-\sigma}$. The dominant $t_{jk}^{\sigma-\sigma}$ connecting a given site $j\sigma$ to sites k-σ will clearly depend strongly on $\epsilon_{j\sigma}$. In the strong coupling regime of primary interest, the dominant such $t_{jk}^{\sigma-\sigma}$ will be those for which $\epsilon_{j\sigma}$ is close to the crossing region (sec. III A); with the largest $t_{jk}^{\sigma-\sigma}$ for $\epsilon_{k-\sigma} \simeq \epsilon_{j\sigma}$, and the $t_{jk}^{\sigma-\sigma}$s decreasing in magnitude as $\epsilon_{k-\sigma}$ is moved away from this region, i.e. as $|\tilde{\xi}_{k-\sigma}| = |\epsilon_{k-\sigma} - \epsilon_{j\sigma}|$ increases from zero. [Note in passing therefore that the dominant sites k-σ connected under $t_{jk}^{\sigma-\sigma}$ to a given site $j\sigma$, will not in general[8] contain the same number of quanta $n_{0-\sigma}^{(k)}$ in their shifted 0-oscillator as $j\sigma$ does in its ($n_{0\sigma}^{(j)}$); in otherwords the relevant sites k-σ in the $-\sigma$-BL will not typically be those lying *directly* above site $j\sigma$ in the σ-BL.]

To formalise the above, write

$$\epsilon_{k-\sigma} \;=\; \epsilon_{j\sigma} \;+\; \tilde{\xi}_{k-\sigma} \tag{60}$$

where the range of $\tilde{\xi}_{k-\sigma}$ reflects the energetic width of the k-σ sites coupled to $j\sigma$ under $t_{jk}^{\sigma-\sigma}$; and

$$t_{jk}^{\sigma-\sigma} \;\equiv\; t_{jk}(\epsilon_{j\sigma};\tilde{\xi}_{k-\sigma}) \tag{61}$$

embodying the fact that $t_{jk}^{\sigma-\sigma}$ depends on $\epsilon_{j\sigma}$ and $\tilde{\xi}_{k-\sigma}$. The $\tilde{\xi}_{k-\sigma}$ are then characterised by a distribution $\tilde{P}(\tilde{\xi}_{k-\sigma})$ (naturally independent of σ for the case $\omega_{0\sigma} = \omega_0$ of primary interest). This reflects the energetic range of the $\epsilon_{k-\sigma}$'s for sites k-σ connected to $j\sigma$ under $t_{jk}^{\sigma-\sigma}$ (rather than intrinsic randomness/stochasticity). As above $\tilde{P}(\tilde{\xi}_{k-\sigma})$ will be peaked around $\tilde{\xi}_{k-\sigma} \simeq 0$, and we expect it to be distributed roughly symmetrically about its maximum.

With the specifications above, eq. 56 can be written as

$$S_{j\sigma}(E) \;=\sum_l{}' \frac{|V_{jl}^{\sigma\sigma}|^2}{E^+ - \epsilon_{j\sigma} - \xi_{l\sigma} - S_{l\sigma}(E)} \;+\; \sum_k \frac{|t_{jk}(\epsilon_{j\sigma};\tilde{\xi}_{k-\sigma})|^2}{E^+ - \epsilon_{j\sigma} - \tilde{\xi}_{k-\sigma} - S_{k-\sigma}(E)} \tag{62}$$

(with the self-energies $S_{n\sigma}(E) = E_{n\sigma}(E) - i\Delta_{n\sigma}(E)$ as usual).

We now proceed in direct parallel to LW §III, within which description the conditional probability distribution $F_\sigma(E_{n\sigma}, \Delta_{n\sigma}; \epsilon_{n\sigma})$ for the real and imaginary parts of the self-energy, given $\epsilon_{n\sigma}$, is the same for all sites n of given σ; i.e. is the same function of $E_{n\sigma}, \Delta_{n\sigma}$ and $\epsilon_{n\sigma}$. That this distribution may however depend on σ is self-evident – it will clearly do so if e.g. the distributions $g_\sigma(V_{jl}^{\sigma\sigma})$ are distinct. Whether or not a state of energy E is localized is then one of self-consistency, by requiring that the above distributions for the self-energies appearing on either side of eq. 62 be self-consistently determined. To render this tractable in practice, we first define the conditional distribution $f_\sigma(\Delta_{n\sigma}; \epsilon_{n\sigma})$ for $\Delta_{n\sigma}$ given $\epsilon_{n\sigma}$ by

$$f_\sigma(\Delta_{n\sigma}; \epsilon_{n\sigma}) \;=\; \int_{-\infty}^{\infty} dE_{n\sigma}\; F_\sigma(E_{n\sigma}, \Delta_{n\sigma}; \epsilon_{n\sigma}) \;. \tag{63}$$

For given E and $\epsilon_{n\sigma}$, the most probable value obtained from this distribution is denoted $\Delta_{\mathrm{mp};\sigma}(E; \epsilon_{n\sigma})$. Referring to eq. 62 for $S_{j\sigma}(E)$, we will typically be interested in eigenvalues E lying close to the unperturbed site energy $\epsilon_{j\sigma}$ of the ('doorway') site $j\sigma$. Here, the dominant perturbative couplings contributing to the rhs of eq. 62 arise from sites $l\sigma$ and k-σ for which $\xi_{l\sigma} \simeq 0 \simeq \tilde{\xi}_{k-\sigma}$, i.e. near-resonant sites for which $\epsilon_{l\sigma} \simeq \overline{\epsilon}_{l\sigma} \simeq \epsilon_{j\sigma}$ and $\epsilon_{k-\sigma} \simeq \overline{\epsilon}_{k-\sigma} \simeq \epsilon_{j\sigma}$ (the overbar denotes an average). In view of this, as in LW, we approximate the imaginary parts of the self-energies of the neighboring sites $l\sigma$ and k-σ by their most probable values, $\Delta_{\mathrm{mp};\sigma}(E; \epsilon_{j\sigma})$ and $\Delta_{\mathrm{mp};-\sigma}(E; \epsilon_{j\sigma})$ respectively. With this, and defining

$$\mu_\sigma \;=\; \eta \;+\; \Delta_{\mathrm{mp};\sigma}(E; \epsilon_{j\sigma}) \tag{64}$$

(for either $\sigma = \uparrow/\downarrow$), eq. 62 gives the following expressions for $E_{j\sigma}$ and $\Delta_{j\sigma}$:

$$E_{j\sigma} \;=\sum_l{}' |V_{jl}^{\sigma\sigma}|^2\; X_{l\sigma} \;+\; \sum_k |t_{jk}(\epsilon_{j\sigma};\tilde{\xi}_{k-\sigma})|^2\; \tilde{X}_{k-\sigma} \tag{65a}$$

$$\Delta_{j\sigma} \;=\sum_l{}' |V_{jl}^{\sigma\sigma}|^2\; Y_{l\sigma} \;+\; \sum_k |t_{jk}(\epsilon_{j\sigma};\tilde{\xi}_{k-\sigma})|^2\; \tilde{Y}_{k-\sigma} \tag{65b}$$

where

$$X_{l\sigma} \;=\; \frac{(E - \epsilon_{j\sigma} - \xi_{l\sigma} - E_{l\sigma})}{(E - \epsilon_{j\sigma} - \xi_{l\sigma} - E_{l\sigma})^2 \;+\; \mu_\sigma^2} \qquad \tilde{X}_{k-\sigma} \;=\; \frac{(E - \epsilon_{j\sigma} - \tilde{\xi}_{k-\sigma} - E_{k-\sigma})}{(E - \epsilon_{j\sigma} - \tilde{\xi}_{k-\sigma} - E_{k-\sigma})^2 \;+\; \mu_{-\sigma}^2} \tag{66a}$$

$$Y_{l\sigma} \;=\; \frac{\mu_\sigma}{(E - \epsilon_{j\sigma} - \xi_{l\sigma} - E_{l\sigma})^2 \;+\; \mu_\sigma^2} \qquad \tilde{Y}_{k-\sigma} \;=\; \frac{\mu_{-\sigma}}{(E - \epsilon_{j\sigma} - \tilde{\xi}_{k-\sigma} - E_{k-\sigma})^2 \;+\; \mu_{-\sigma}^2}\;. \tag{66b}$$

From eqs. 66, using the distributions $g_\sigma(V^{\sigma\sigma})$, $P_\sigma(\xi)$, $\tilde{P}(\tilde{\xi})$, an explicit functional form for the $f_\sigma(\Delta_{j\sigma}; \epsilon_{j\sigma})$ (with $\sigma = \uparrow/\downarrow$) will be obtained; from which self-consistency is subsequently enforced by requiring that its most probable value be equal to the input most probable values $\Delta_{\mathrm{mp};\sigma}(E; \epsilon_{j\sigma})$ entering the μ_σ above. This we now consider, in analogy to LW eqs. (20) *ff.*

With the above procedure, $F_\sigma(E_{j\sigma},\Delta_{j\sigma};\epsilon_{j\sigma})$ is given by

$$\begin{aligned} F_\sigma(E_{j\sigma},\Delta_{j\sigma};\epsilon_{j\sigma}) \;=\; & \int\cdot\cdot\int \prod_l \left[dE_{l\sigma}d\Delta_{l\sigma}d\xi_{l\sigma}dV_{jl}^{\sigma\sigma}F_\sigma(E_{l\sigma},\Delta_{l\sigma};\epsilon_{j\sigma}+\xi_{l\sigma})P_\sigma(\xi_{l\sigma})g_\sigma(V_{jl}^{\sigma\sigma})\right] \\ & \times \prod_k \left[dE_{k-\sigma}d\Delta_{k-\sigma}d\tilde{\xi}_{k-\sigma}F_{-\sigma}(E_{k-\sigma},\Delta_{k-\sigma};\epsilon_{j\sigma}+\tilde{\xi}_{k-\sigma})\tilde{P}(\tilde{\xi}_{k-\sigma})\right] \\ & \times \delta\left(E_{j\sigma}-{\sum_l}'|V_{jl}^{\sigma\sigma}|^2\;X_{l\sigma}-\sum_k |t_{jk}(\epsilon_{j\sigma};\tilde{\xi}_{k-\sigma})|^2\;\tilde{X}_{k-\sigma}\right) \\ & \times \delta\left(\Delta_{j\sigma}-{\sum_l}'|V_{jl}^{\sigma\sigma}|^2\;Y_{l\sigma}-\sum_k |t_{jk}(\epsilon_{j\sigma};\tilde{\xi}_{k-\sigma})|^2\;\tilde{Y}_{k-\sigma}\right) \end{aligned} \tag{67}$$

(where from now on all integration limits are $\pm\infty$ unless specified otherwise). Now define the conditional distribution for $E_{n\sigma}$ given $\epsilon_{n\sigma}$,

$$f_{0\sigma}(E_{n\sigma};\epsilon_{n\sigma}) \;=\; \int d\Delta_{n\sigma}\;F_\sigma(E_{n\sigma},\Delta_{n\sigma};\epsilon_{n\sigma}). \tag{68}$$

Recognising that the $X_{l\sigma}$ and $Y_{l\sigma}$ do not depend on the $\Delta_{l\sigma}$, and that the $\tilde{X}_{k-\sigma}$ and $\tilde{Y}_{k-\sigma}$ are independent of the $\Delta_{k-\sigma}$, eq. 67 may be integrated over $\Delta_{j\sigma}$ to give

$$\begin{aligned} f_{0\sigma}(E_{j\sigma};\epsilon_{j\sigma}) \;=\; & \int\cdot\cdot\int \prod_l \left[dE_{l\sigma}d\xi_{l\sigma}dV_{jl}^{\sigma\sigma}\;f_{0\sigma}(E_{l\sigma};\epsilon_{j\sigma}+\xi_{l\sigma})P_\sigma(\xi_{l\sigma})g_\sigma(V_{jl}^{\sigma\sigma})\right] \\ & \times \prod_k \left[dE_{k-\sigma}d\tilde{\xi}_{k-\sigma}\;f_{0-\sigma}(E_{k-\sigma};\epsilon_{j\sigma}+\tilde{\xi}_{k-\sigma})\tilde{P}(\tilde{\xi}_{k-\sigma})\right] \\ & \times \delta\left(E_{j\sigma}-{\sum_l}'|V_{jl}^{\sigma\sigma}|^2\;X_{l\sigma}-\sum_k |t_{jk}(\epsilon_{j\sigma};\tilde{\xi}_{k-\sigma})|^2\;\tilde{X}_{k-\sigma}\right) \end{aligned} \tag{69}$$

(which form closed integral equations for the conditional distributions $f_{0\sigma}(E_{n\sigma};\epsilon_{n\sigma})$, $\sigma=\uparrow/\downarrow$).

By the same token – but more importantly – integrating eq. 67 over $E_{j\sigma}$ gives

$$\begin{aligned} f_\sigma(\Delta_{j\sigma};\epsilon_{j\sigma}) \;=\; & \int\cdot\cdot\int \prod_l \left[dE_{l\sigma}d\xi_{l\sigma}dV_{jl}^{\sigma\sigma}\;f_{0\sigma}(E_{l\sigma};\epsilon_{j\sigma}+\xi_{l\sigma})P_\sigma(\xi_{l\sigma})g_\sigma(V_{jl}^{\sigma\sigma})\right] \\ & \times \prod_k \left[dE_{k-\sigma}d\tilde{\xi}_{k-\sigma}\;f_{0-\sigma}(E_{k-\sigma};\epsilon_{j\sigma}+\tilde{\xi}_{k-\sigma})\tilde{P}(\tilde{\xi}_{k-\sigma})\right] \\ & \times \delta\left(\Delta_{j\sigma}-{\sum_l}'|V_{jl}^{\sigma\sigma}|^2\;Y_{l\sigma}-\sum_k |t_{jk}(\epsilon_{j\sigma};\tilde{\xi}_{k-\sigma})|^2\;\tilde{Y}_{k-\sigma}\right)\;. \end{aligned} \tag{70}$$

With the $f_{0\sigma}$ known from solution of eq. 69, eq. 70 constitutes an explicit functional form for $f_\sigma(\Delta_{j\sigma};\epsilon_{j\sigma})$; from which self-consistency can then be enforced as sketched above. To analyze this further we take the Fourier transform[9]

$$\hat{f}_\sigma(k;\epsilon_{j\sigma}) \;=\; \int_{-\infty}^{\infty} d\Delta_{j\sigma}\quad e^{ik\Delta_{j\sigma}}f_\sigma(\Delta_{j\sigma};\epsilon_{j\sigma}) \tag{71a}$$

$$\Longrightarrow\quad f_\sigma(\Delta_{j\sigma};\epsilon_{j\sigma}) \;=\; \int_{-\infty}^{\infty}\frac{dk}{2\pi}\quad e^{-ik\Delta_{j\sigma}}\hat{f}_\sigma(k;\epsilon_{j\sigma})\;. \tag{71b}$$

Eq. 71a used in eq. 70 then gives

$$\begin{aligned} \hat{f}_\sigma(k;\epsilon_{j\sigma}) \;=\; & \int\cdot\cdot\int \prod_l \left[dE_{l\sigma}d\xi_{l\sigma}dV_{jl}^{\sigma\sigma}\;f_{0\sigma}(E_{l\sigma};\epsilon_{j\sigma}+\xi_{l\sigma})P_\sigma(\xi_{l\sigma})g_\sigma(V_{jl}^{\sigma\sigma})\right] \\ & \times \prod_k \left[dE_{k-\sigma}d\tilde{\xi}_{k-\sigma}\;f_{0-\sigma}(E_{k-\sigma};\epsilon_{j\sigma}+\tilde{\xi}_{k-\sigma})\tilde{P}(\tilde{\xi}_{k-\sigma})\right] \\ & \times \exp\left(ik{\sum_l}'|V_{jl}^{\sigma\sigma}|^2\;Y_{l\sigma}\right)\exp\left(ik\sum_k |t_{jk}(\epsilon_{j\sigma};\tilde{\xi}_{k-\sigma})|^2\;\tilde{Y}_{k-\sigma}\right) \end{aligned} \tag{72}$$

which is clearly separable, of form

$$\hat{f}_\sigma(k;\epsilon_{j\sigma}) \;=\; \hat{f}_{V\sigma}(k;\epsilon_{j\sigma}) \times \hat{f}_{t\sigma}(k;\epsilon_{j\sigma}) \tag{73a}$$

$$\Longrightarrow \quad f_\sigma(\Delta_{j\sigma};\epsilon_{j\sigma}) \;=\; \int_{-\infty}^{\infty} d\Delta \; \hat{f}_{V\sigma}(\Delta_{j\sigma}-\Delta;\epsilon_{j\sigma})\hat{f}_{t\sigma}(\Delta;\epsilon_{j\sigma}) \tag{73b}$$

with

$$\hat{f}_{V\sigma}(k;\epsilon_{j\sigma}) = \left[\int dE_{l\sigma}d\xi dV \; f_{0\sigma}(E_{l\sigma};\epsilon_{j\sigma}+\xi)P_\sigma(\xi)g_\sigma(V) \; \exp\left(\frac{ik\;|V|^2\mu_\sigma}{[E-\epsilon_{j\sigma}-\xi-E_{l\sigma}]^2 \;+\; \mu_\sigma^2}\right)\right]^K \tag{74a}$$

$$\hat{f}_{t\sigma}(k;\epsilon_{j\sigma}) = \left[\int dE_{k-\sigma}d\tilde{\xi} \; f_{0-\sigma}(E_{k-\sigma};\epsilon_{j\sigma}+\tilde{\xi})\tilde{P}(\tilde{\xi}_{k-\sigma}) \; \exp\left(\frac{ik\;|t(\epsilon_{j\sigma};\tilde{\xi})|^2\mu_{-\sigma}}{[E-\epsilon_{j\sigma}-\tilde{\xi}-E_{k-\sigma}]^2 \;+\; \mu_{-\sigma}^2}\right)\right]^{K_t} \tag{74b}$$

(recall that K is the number of sites $l\sigma$ to which site $j\sigma$ is coupled under $V_{jl}^{\sigma\sigma}$, and K_t is similarly the number of sites k-σ to which it is coupled under $t_{jk}^{\sigma-\sigma}$). Equivalently, since the distributions $f_{0\sigma}, P_\sigma, g_\sigma$ and $\tilde{P}$ are all normalized to unity, can eq.74 can be written as

$$\hat{f}_{V\sigma}(k;\epsilon_{j\sigma}) = \left[1+\int dE_{l\sigma}d\xi dV \; f_{0\sigma}(E_{l\sigma};\epsilon_{j\sigma}+\xi)P_\sigma(\xi)g_\sigma(V) \; \left(\exp\left[\frac{ik\;|V|^2\mu_\sigma}{(E-\epsilon_{j\sigma}-\xi-E_{l\sigma})^2 \;+\; \mu_\sigma^2}\right]-1\right)\right]^K \tag{75a}$$

$$\hat{f}_{t\sigma}(k;\epsilon_{j\sigma}) = \left[1+\int dE_{k-\sigma}d\tilde{\xi} \; f_{0-\sigma}(E_{k-\sigma};\epsilon_{j\sigma}+\tilde{\xi})\tilde{P}(\tilde{\xi}) \; \left(\exp\left[\frac{ik\;|t(\epsilon_{j\sigma};\tilde{\xi})|^2\mu_{-\sigma}}{(E-\epsilon_{j\sigma}-\tilde{\xi}-E_{k-\sigma})^2 \;+\; \mu_{-\sigma}^2}\right]-1\right)\right]^{K_t} . \tag{75b}$$

Eqs. 75 (with eq. 73) are the basic equations to analyze; and note that for $H_t \equiv 0$ (i.e. $t(\epsilon_{j\sigma};\tilde{\xi})=0$) they give $\hat{f}_{t\sigma}(k;\epsilon_{j\sigma})=1$, and reduce precisely to eq. (23) of LW. We return to them below. First, however, we consider the physical interpretation of several functions which will arise in our subsequent analysis.

A. Local densities of states

At the most probable value level of description, and for a given realization, the local Green function for site $l\sigma$ connected to site $j\sigma$ under $V_{jl}^{\sigma\sigma}$ is simply $G_{l\sigma}(E) \simeq [E-\epsilon_{l\sigma}-E_{l\sigma}+i\mu_\sigma]^{-1} \equiv [E-\epsilon_{j\sigma}-\xi-E_{l\sigma}+i\mu_\sigma]^{-1}$. The corresponding local density of states (LDoS), denoted $N_{l\sigma}(E) \equiv N_{l\sigma}(E;E_{l\sigma};\epsilon_{j\sigma}+\xi)$, is thus

$$N_{l\sigma}(E;E_{l\sigma};\epsilon_{j\sigma}+\xi) \;=\; -\tfrac{1}{\pi}\mathrm{Im}G_{l\sigma}(E) \;=\; \frac{\mu_\sigma/\pi}{(E-\epsilon_{j\sigma}-\xi-E_{l\sigma})^2+\mu_\sigma^2} \tag{76}$$

and depends upon the random variables $E_{l\sigma}$ and ξ. Averaging over the probability distribution for the former gives the partially averaged LDoS denoted $\overline{N}_{l\sigma}(E;\epsilon_{j\sigma}+\xi) \equiv \langle N_{l\sigma}(E)\rangle_{E_{l\sigma}}$, *viz*

$$\overline{N}_{l\sigma}(E;\epsilon_{j\sigma}+\xi) \;=\; \int dE_{l\sigma} \; f_{0\sigma}(E_{l\sigma};\epsilon_{j\sigma}+\xi) \; N_{l\sigma}(E;E_{l\sigma};\epsilon_{j\sigma}+\xi); \tag{77}$$

and averaging this over $P_\sigma(\xi)$ then gives the fully averaged LDoS, denoted $D_{L\sigma}(E;\epsilon_{j\sigma}) \equiv \langle N_{l\sigma}(E)\rangle_{E_{l\sigma},\xi}$, i.e.

$$D_{L\sigma}(E;\epsilon_{j\sigma}) \;=\; \int d\xi \; P_\sigma(\xi)\overline{N}_{l\sigma}(E;\epsilon_{j\sigma}+\xi) \; . \tag{78}$$

Let me emphasize here that eqs. 76-78 – and in particular eq. 78 for $D_{L\sigma}(E;\epsilon_{j\sigma})$ – are quite general, and not e.g. confined to the localized limit where $\mu_\sigma \propto \eta \to 0+$. In LW by contrast, $D_{L\sigma}(E;\epsilon_{j\sigma})$ (there without the need for a σ label) is used to refer exclusively to the localized regime (as in eq. 83 below). Note further that with the substitution $-x = E-\epsilon_{j\sigma}-\xi-E_{l\sigma}$ in eq. 77 (such that $dE_{l\sigma} \equiv dx$),

$$\overline{N}_{l\sigma}(E;\epsilon_{j\sigma}+\xi) \;=\; \int dx \; f_{0\sigma}(E-\epsilon_{j\sigma}-\xi+x;\epsilon_{j\sigma}+\xi) \; \frac{\mu_\sigma/\pi}{x^2+\mu_\sigma^2} \tag{79}$$

and hence $D_{L\sigma}(E;\epsilon_{j\sigma})$ may be expressed alternatively as

$$D_{L\sigma}(E;\epsilon_{j\sigma}) \;=\; \int dx\; M_\sigma(x;E;\epsilon_{j\sigma})\;\frac{\mu_\sigma/\pi}{x^2+\mu_\sigma^2}\;; \tag{80}$$

where

$$M_\sigma(x;E;\epsilon_{j\sigma}) \;=\; \int d\xi\; f_{0\sigma}(E-\epsilon_{j\sigma}-\xi+x;\epsilon_{j\sigma}+\xi)\;P_\sigma(\xi) \tag{81}$$

is thus defined, and is normalized to unity,

$$\int dx\; M_\sigma(x;E;\epsilon_{j\sigma}) \;=\; 1 \tag{82}$$

(since $\int d\xi\;P_\sigma(\xi)=1=\int dy\;f_{0\sigma}(y;\epsilon_{j\sigma}+\xi)$ are separately normalized). Eq. 80 is of course quite general, as noted above; but for the particular case where states of energy E are localized, i.e. $\mu_\sigma\to 0+$, it reduces to

$$D_{L\sigma}(E;\epsilon_{j\sigma}) \;=\; M_\sigma(x=0;E;\epsilon_{j\sigma}) \qquad :\ \text{localized states} \tag{83}$$

as will be employed in later sections.

Directly analogous results follow for the local Green function for site k-σ connected to site $j\sigma$ under $t_{jk}^{\sigma-\sigma}$; given at most probable value level by $G_{k-\sigma}(E)\simeq[E-\epsilon_{k-\sigma}-E_{k-\sigma}+i\mu_{-\sigma}]^{-1}$ but where now $\epsilon_{k-\sigma}=\epsilon_{j\sigma}+\tilde{\xi}$, and hence $G_{k-\sigma}(E)\equiv[E-\epsilon_{j\sigma}-\tilde{\xi}-E_{k-\sigma}+i\mu_{-\sigma}]^{-1}$. In particular (as in eq. 77),

$$\overline{N}_{k-\sigma}(E;\epsilon_{j\sigma}+\tilde{\xi}) \;=\; \int dE_{k-\sigma}\; f_{0-\sigma}(E_{k-\sigma};\epsilon_{j\sigma}+\tilde{\xi})N_{k-\sigma}(E;E_{k-\sigma};\epsilon_{j\sigma}+\tilde{\xi}) \tag{84}$$

where (*cf* eq. 76)

$$N_{k-\sigma}(E;E_{k-\sigma};\epsilon_{j\sigma}+\tilde{\xi}) \;=\; \frac{\mu_{-\sigma}/\pi}{(E-\epsilon_{j\sigma}-\tilde{\xi}-E_{k-\sigma})^2+\mu_{-\sigma}^2}\;; \tag{85}$$

or equivalently (using $-x=E-\epsilon_{j\sigma}-\tilde{\xi}-E_{k-\sigma}$ in eq. 84)

$$\overline{N}_{k-\sigma}(E;\epsilon_{j\sigma}+\tilde{\xi}) \;=\; \int dx\; f_{0-\sigma}(E-\epsilon_{j\sigma}-\tilde{\xi}+x;\epsilon_{j\sigma}+\tilde{\xi})\;\frac{\mu_{-\sigma}/\pi}{x^2+\mu_{-\sigma}^2}\;. \tag{86}$$

In analogy to eq. 78, the average of $\overline{N}_{k-\sigma}(E;\epsilon_{j\sigma}+\tilde{\xi})$ over the distribution $\tilde{P}(\tilde{\xi})$ of $\tilde{\xi}$ is denoted $\tilde{D}_{L-\sigma}(E;\epsilon_{j\sigma})$, i.e.

$$\tilde{D}_{L-\sigma}(E;\epsilon_{j\sigma}) \;=\; \int d\tilde{\xi}\;\tilde{P}(\tilde{\xi})\;\overline{N}_{k-\sigma}(E;\epsilon_{j\sigma}+\tilde{\xi}) \tag{87}$$

Although eq. 84 is the precise analogue of eq. 77, note that – since the distributions $P_\sigma(\xi)$ and $\tilde{P}(\tilde{\xi})$ are physically quite distinct – $\tilde{D}_{L-\sigma}(E;\epsilon_{j\sigma})$ is *not* of course the same as $D_{L-\sigma}(E;\epsilon_{j-\sigma})$ of eq. 78 (for $-\sigma$).

For later use, we also define average powers of $t_{jk}^{\sigma-\sigma}\equiv t(\epsilon_{j\sigma};\tilde{\xi})$ by $\langle|t|^m\rangle=\int d\tilde{\xi}\;W(\tilde{\xi})\;|t(\epsilon_{j\sigma};\tilde{\xi})|^m/\int d\tilde{\xi}\;W(\tilde{\xi})$ with the measure $W(\tilde{\xi})=\tilde{P}(\tilde{\xi})\overline{N}_{k-\sigma}(E;\epsilon_{j\sigma}+\tilde{\xi})$, i.e.

$$\langle|t|^m\rangle \;=\; \frac{\int d\tilde{\xi}\;\tilde{P}(\tilde{\xi})\;\overline{N}_{k-\sigma}(E;\epsilon_{j\sigma}+\tilde{\xi})\;|t(\epsilon_{j\sigma};\tilde{\xi})|^m}{\int d\tilde{\xi}\;\tilde{P}(\tilde{\xi})\;\overline{N}_{k-\sigma}(E;\epsilon_{j\sigma}+\tilde{\xi})} \;\equiv\; \frac{\int d\tilde{\xi}\;\tilde{P}(\tilde{\xi})\;\overline{N}_{k-\sigma}(E;\epsilon_{j\sigma}+\tilde{\xi})\;|t(\epsilon_{j\sigma};\tilde{\xi})|^m}{\tilde{D}_{L-\sigma}(E;\epsilon_{j\sigma})}\;. \tag{88}$$

Note in particular that for a regime of localized states, for which $\mu_{-\sigma}\to 0$ and hence $N_{k-\sigma}(E;E_{k-\sigma};\epsilon_{j\sigma}+\tilde{\xi})=\delta(E-\epsilon_{j\sigma}-\tilde{\xi}-E_{k-\sigma})$ (eq. 85), we have (eq. 84) $\overline{N}_{k-\sigma}(E;\epsilon_{j\sigma}+\tilde{\xi})=f_{0-\sigma}(E-\epsilon_{j\sigma}-\tilde{\xi};\epsilon_{j\sigma}+\tilde{\xi})$. Eq. 87 then reduces to

$$\tilde{D}_{L-\sigma}(E;\epsilon_{j\sigma}) \;=\; \int d\tilde{\xi}\;\tilde{P}(\tilde{\xi})\;f_{0-\sigma}(E-\epsilon_{j\sigma}-\tilde{\xi};\epsilon_{j\sigma}+\tilde{\xi}) \qquad :\ \text{localized states} \tag{89}$$

and eq. 88 becomes

$$\langle|t|^m\rangle \;=\; \frac{\int d\tilde{\xi}\;\tilde{P}(\tilde{\xi})\;f_{0-\sigma}(E-\epsilon_{j\sigma}-\tilde{\xi};\epsilon_{j\sigma}+\tilde{\xi})\;|t(\epsilon_{j\sigma};\tilde{\xi})|^m}{\int d\tilde{\xi}\;\tilde{P}(\tilde{\xi})\;f_{0-\sigma}(E-\epsilon_{j\sigma}-\tilde{\xi};\epsilon_{j\sigma}+\tilde{\xi})} \qquad :\ \text{localized states}\;. \tag{90}$$

B. Initial overview

The basic self-consistency equations are eqs. 75. Equivalently, with the substitution $-x = E - \epsilon_{j\sigma} - \xi - E_{l\sigma}$ in eq. 75a, and $-x = E - \epsilon_{j\sigma} - \tilde{\xi} - E_{k-\sigma}$ in eq. 75b, these reduce to

$$\hat{f}_{V\sigma}(k;\epsilon_{j\sigma}) = \left[1 + \int dV \int dx\ g_\sigma(V) M_\sigma(x;E;\epsilon_{j\sigma})\ \left(\exp\left[\frac{ik\ |V|^2\mu_\sigma}{x^2\ +\ \mu_\sigma^2}\right] - 1\right)\right]^K \tag{91a}$$

$$\hat{f}_{t\sigma}(k;\epsilon_{j\sigma}) = \left[1 + \int d\tilde{\xi} \int dx\ f_{0-\sigma}(E - \epsilon_{j\sigma} - \tilde{\xi} + x; \epsilon_{j\sigma} + \tilde{\xi})\tilde{P}(\tilde{\xi})\ \left(\exp\left[\frac{ik\ |t(\epsilon_{j\sigma};\tilde{\xi})|^2\mu_{-\sigma}}{x^2\ +\ \mu_{-\sigma}^2}\right] - 1\right)\right]^{K_t} \tag{91b}$$

with $M_\sigma(x;E;\epsilon_{j\sigma})$ given by eq. 81.

Now let's get an initial overview of these equations. First, recall some familiar basic properties of the Fourier transform eq. 71 for $\hat{f}_\sigma(k) \equiv \hat{f}_\sigma(k;\epsilon_{j\sigma})$ (temporarily dropping the $\epsilon_{j\sigma}$-dependence for brevity). From eq. 71a, $\hat{f}_\sigma(k=0) = \int_{-\infty}^{\infty} d\Delta_\sigma\ f_\sigma(\Delta_\sigma) = 1$, since the distribution is normalized to unity (similarly $\hat{f}_{V\sigma}(k=0) = 1 = \hat{f}_{t\sigma}(k=0)$ as follows directly from eq. 91). Likewise from eq. 71a (and remembering that $f_\sigma(\Delta_\sigma) \neq 0$ only for $\Delta_\sigma \geq 0$)

$$-i\left(\frac{\partial \hat{f}_\sigma(k)}{\partial k}\right)_{k=0} \quad = \quad \int_0^\infty d\Delta_\sigma\ \Delta_\sigma f_\sigma(\Delta_\sigma)\ \equiv\ \langle\Delta_\sigma\rangle \tag{92}$$

gives the mean value of Δ_σ ($\equiv \Delta_{j\sigma}$). Consider then the leading $k \to 0$ behavior[10] of $\hat{f}_\sigma(k)$,

$$\hat{f}_\sigma(k)\ \ \overset{k\to 0}{\sim}\ \ 1\ +\ c\ k^\gamma\ . \tag{93}$$

Since $\hat{f}_\sigma(k=0) = 1$, the exponent $\gamma > 0$ necessarily. If $0 < \gamma < 1$, then $(\partial \hat{f}_\sigma(k)/\partial k)_{k=0}$ diverges, so the mean $\langle\Delta_\sigma\rangle$ is divergent, eq. 92. The latter is the behavior expected for a regime of localized states – or more precisely it is expected for the distribution of $\Delta_\sigma(E)/\eta$ in this regime (see sec. V) – so in that case we expect $\gamma < 1$; that this indeed arises from eqs. 75 or 91 will be shown in sec. V.

If by contrast $\gamma = 1$ in eq. 93, then the mean $\langle\Delta_\sigma\rangle$ is non-zero and finite. This is the behavior characteristic of a regime of extended states, so let's consider it. From eq. 92 and eq. 73a,

$$\langle\Delta_\sigma\rangle \quad = \quad -\ i\left(\frac{\partial \hat{f}_{V\sigma}(k)}{\partial k}\right)_{k=0}\ -\ i\left(\frac{\partial \hat{f}_{t\sigma}(k)}{\partial k}\right)_{k=0} \tag{94}$$

(since $\hat{f}_{V\sigma}(k=0) = 1 = \hat{f}_{t\sigma}(k=0)$). Now consider eqs. 91 for $\hat{f}_{V\sigma}(k)$ and $\hat{f}_{t\sigma}(k)$, for the case corresponding to extended states where μ_σ ($= \eta + \Delta_{\mathrm{mp};\sigma}(E;\epsilon_{j\sigma})$) is finite for both σ. [Note incidentally that because $\mu_\sigma > 0$ (and $\mu_{-\sigma} > 0$) here, the exponentials in eq. 91 can each legitimately be expanded to leading linear order in k; but that this would *not* be the case if $\mu_\sigma \propto \eta \to 0$, as we shall see later when consider the regime of localized states.] From eq. 91a, we have

$$-i\left(\frac{\partial \hat{f}_{V\sigma}(k)}{\partial k}\right)_{k=0} \quad = K\ \langle|V^{\sigma\sigma}|^2\rangle\ \int dx\ M_\sigma(x;\epsilon_{j\sigma})\frac{\mu_\sigma}{x^2+\mu_\sigma^2} \tag{95a}$$

$$= \pi K\ \langle|V^{\sigma\sigma}|^2\rangle\ D_{L\sigma}(E;\epsilon_{j\sigma}) \tag{95b}$$

(from eq. 78 for the averaged LDoS $D_{L\sigma}(E;\epsilon_{j\sigma})$); where

$$\langle|V^{\sigma\sigma}|^2\rangle \quad = \quad \int dV\ g_\sigma(V)\ |V|^2 \tag{96}$$

in obvious notation. Now consider $(\partial \hat{f}_{t\sigma}(k)/\partial k)_{k=0}$. From eq. 91b,

$$-i\left(\frac{\partial \hat{f}_{t\sigma}(k)}{\partial k}\right)_{k=0} \quad = \pi K_t\ \int d\tilde{\xi} \int dx\ \tilde{P}(\tilde{\xi}) f_{0-\sigma}(E - \epsilon_{j\sigma} - \tilde{\xi} + x; \epsilon_{j\sigma} + \tilde{\xi})\ |t(\epsilon_{j\sigma};\tilde{\xi})|^2\ \frac{\mu_{-\sigma}/\pi}{x^2+\mu_{-\sigma}^2} \tag{97a}$$

$$= \pi K_t\ \int d\tilde{\xi}\ \tilde{P}(\tilde{\xi})\ \overline{N}_{k-\sigma}(E;\epsilon_{j\sigma}+\tilde{\xi})\ |t(\epsilon_{j\sigma};\tilde{\xi})|^2 \tag{97b}$$

on using eq. 86; and hence from eq. 88,

$$-i\left(\frac{\partial \hat{f}_{t\sigma}(k)}{\partial k}\right)_{k=0} = \pi K_t \ \langle |t|^2\rangle \ \tilde{D}_{L-\sigma}(E;\epsilon_{j\sigma}) \ . \tag{98}$$

Eqs. 94,95b,98 thus give the desired result for the mean value

$$\langle \Delta_\sigma\rangle \ = \ \pi K \ \langle |V^{\sigma\sigma}|^2\rangle \ D_{L\sigma}(E;\epsilon_{j\sigma}) \ + \ \pi K_t \ \langle |t|^2\rangle \ \tilde{D}_{L-\sigma}(E;\epsilon_{j\sigma}) \tag{99}$$

in a regime of delocalized states.

We return to this shortly, but first consider the variance of Δ_σ, $\langle(\delta\Delta_\sigma)^2\rangle = \langle(\Delta_\sigma - \langle\Delta_\sigma\rangle)^2\rangle$. From eq. 71a, $\langle\Delta_\sigma^2\rangle = -(\partial^2\hat{f}_\sigma(k)/\partial k^2)_{k=0}$ and $\langle\Delta_\sigma\rangle^2 = -[(\partial\hat{f}_\sigma(k)/\partial k)_{k=0}]^2$; and since $\hat{f}_\sigma(k) = \hat{f}_{V\sigma}(k)\times\hat{f}_{t\sigma}(k)$ (eq. 73a), one obtains

$$\langle(\delta\Delta_\sigma)^2\rangle \ = \ \sum_{\alpha=V,t}\left(-\Big(\frac{\partial^2\hat{f}_{\alpha\sigma}(k)}{\partial k^2}\Big)_{k=0} + \Big[\Big(\frac{\partial\hat{f}_{\alpha\sigma}(k)}{\partial k}\Big)_{k=0}\Big]^2\right) \ \equiv \sum_{\alpha=V,t}\langle(\delta\Delta_{\alpha\sigma})^2\rangle \tag{100}$$

(i.e. a sum of the separate variances, as expected). From eq. 91, each $\hat{f}_{\alpha\sigma}(k)$ is of form $\hat{f}_{\alpha\sigma}(k) = [I_\alpha(k)]^{K_\alpha}$ with $I_\alpha(k=0)=1$ (and $K_V\equiv K, K_t = K_t$); from which one finds $\langle(\delta\Delta_{\alpha\sigma})^2\rangle = -K_\alpha(\partial^2 I_\alpha(k)/\partial k^2)_{k=0} + K_\alpha[(\partial I_\alpha(k)/\partial k)_{k=0}]^2$, which is readily calculated. Following this procedure, and considering explicitly $\alpha = V$, one obtains

$$\langle(\delta\Delta_{V\sigma})^2\rangle \ = \pi^2 K\left(\langle|V^{\sigma\sigma}|^4\rangle\langle[N_{l\sigma}(E)]^2\rangle_{E_{l\sigma},\xi} \ - \ \Big(\langle|V^{\sigma\sigma}|^2\rangle\langle N_{l\sigma}(E)\rangle_{E_{l\sigma},\xi}\Big)^2\right) \tag{101a}$$

$$\equiv \pi^2 K\left(\langle\Big(|V^{\sigma\sigma}|^2 N_{l\sigma}(E)\Big)^2\rangle \ - \ \Big(\langle|V^{\sigma\sigma}|^2 N_{l\sigma}(E)\rangle\Big)^2\right) \ . \tag{101b}$$

Here $\langle[N_{l\sigma}(E)]^m\rangle_{E_{l\sigma},\xi}$ denotes the fully averaged m^{th} power of the LDoS $N_{l\sigma}(E)\equiv N_{l\sigma}(E;E_{l\sigma};\epsilon_{j\sigma}+\xi) = (\mu_\sigma/\pi)/[(E-\epsilon_{j\sigma}-\xi-E_{l\sigma})^2+\mu_\sigma^2]$ (eq. 76), such that for $m=1$, $\langle N_{l\sigma}(E)\rangle_{E_{l\sigma},\xi} = D_{L\sigma}(E;\epsilon_{j\sigma})$ (eqs. 77,78). It is given by

$$\langle[N_{l\sigma}(E)]^m\rangle_{E_{l\sigma},\xi} \ = \ \int\!\!\int d\xi dE_{l\sigma} \ P_\sigma(\xi) f_{0\sigma}(E_{l\sigma};\epsilon_{j\sigma}+\xi)\left[\frac{\mu_\sigma/\pi}{(E-\epsilon_{j\sigma}-\xi-E_{l\sigma})^2+\mu_\sigma^2}\right]^m \tag{102a}$$

$$= \ \int dx \ M_\sigma(x;E;\epsilon_{j\sigma})\left[\frac{\mu_\sigma/\pi}{x^2+\mu_\sigma^2}\right]^m \tag{102b}$$

(using eq. 81).

Now return to eq. 99 for the mean $\langle\Delta_\sigma\rangle$ in a delocalized regime. It is clearly of golden rule-like form. That was appreciated in LW (see e.g. LW eq. 57, pg 5008 and comments there); at least insofar as taking the average of $\Delta_j(E) = \pi\sum_l' |V_{jl}|^2 N_l(E)$ gives directly the first term on the right side of eq. 99 (although I don't recall appreciating then that our working theory for $\hat{f}(k)\leftrightarrow f(\Delta)$ itself gives this result correctly).

Two further points should be noted here. First, although eq. 99 is of golden rule form, $D_{L\sigma}(E;\epsilon_{j\sigma})$ and $\tilde{D}_{L-\sigma}(E;\epsilon_{j\sigma})$ therein still depend self-consistently on $\mu_\sigma = \eta + \Delta_{\mathrm{mp};\sigma}(E;\epsilon_{j\sigma})$ (for $\sigma = \uparrow/\downarrow$), as they should; although for sufficiently strongly delocalized states we naturally expect $\Delta_{\mathrm{mp};\sigma}(E;\epsilon_{j\sigma})\simeq\langle\Delta_\sigma\rangle$. In the delocalized asymptotic limit $\mu_\sigma\to\infty$, eq. 99 reduces (using $D_{L\sigma}(E;\epsilon_{j\sigma})\to 1/\pi\mu_\sigma$ from eqs. 80,82 and $\tilde{D}_{L-\sigma}(E;\epsilon_{j\sigma})\to 1/\pi\mu_{-\sigma}$ from eqs. 86,87) to

$$\langle\Delta_\sigma\rangle \ \overset{\mu_\sigma\to\infty}{\sim} \ \frac{K\langle|V^{\sigma\sigma}|^2\rangle}{\mu_\sigma} \ + \ \frac{K_t\langle|t|^2\rangle}{\mu_{-\sigma}} \ , \tag{103}$$

which (for $t\equiv t_{jl}^{\sigma-\sigma}=0$) is indeed the estimate of Δ_{mp} used in LW eq. 32. Notice however that even in this limit, eq. 101b for the variance reduces to $\langle(\delta\Delta_{V\sigma})^2\rangle = K\langle\big(|V^{\sigma\sigma}|^2 - \langle|V^{\sigma\sigma}|^2\rangle\big)^2\rangle/\mu_\sigma^2$; so that the ratio of the mean to the standard deviation, $\langle\Delta_\sigma\rangle/[\langle(\delta\Delta_{V\sigma})^2\rangle]^{1/2}$, remains $\mathcal{O}(1)$ and hence fluctuations cannot strictly be ignored.[11]

The second point is perhaps a little more subtle. Look again at eq. 99 and, *using it*, consider the localized regime where $\mu_\sigma\propto\eta\to 0+$ (for both σ). In this case, $D_{L\sigma}(E;\epsilon_{j\sigma})$ and $\tilde{D}_{L-\sigma}(E;\epsilon_{j\sigma})$ both remain finite (see e.g. eq. 83). It would thus appear that $\langle\Delta_\sigma\rangle$ is finite in a regime of localized states, and this indeed is correct: in the localized domain (considered explicitly in sec. V), $\Delta_{j\sigma}(E;\epsilon_{j\sigma})\equiv\Delta_\sigma\propto\eta\to 0+$ with probability unity, but the mean value of Δ_σ/η diverges – corresponding to a finite mean $\langle\Delta_\sigma\rangle$.[12] While the conclusion itself is substantively correct, the argument here is nevertheless somewhat misleading, since eq. 99 itself holds under the assumption that the leading low-k behavior of $\hat{f}_\sigma(k)$ is linear, i.e. the exponent $\gamma = 1$ in eq. 93. As shown in the following section, however, $\gamma = \frac{1}{2}$ in a localized regime; corresponding to a divergent mean for the distribution of Δ_σ/η, and indicative of the fact that the mean value of Δ_σ, finite though it is, is not remotely characteristic of its distribution in such a regime (which is of course the very reason why we focus instead on its most probable value $\Delta_{\mathrm{mp};\sigma}$).

In a regime of extended states the leading low-k behavior of $\hat{f}_\sigma(k)$ *is* however linear, $\langle\Delta_\sigma\rangle$ is finite, and one can legitimately ask for the behavior of $\langle\Delta_\sigma\rangle$ as the localization transition is approached from the extended side. This of course corresponds again to $\mu_\sigma \to 0+$; so again one concludes that $\langle\Delta_\sigma\rangle$ remains finite as the transition is approached. But while the mean approaches a finite value, all other moments of the distribution diverge. This is directly evident from eq. 102b for the m^{th} moment of the LDoS $N_{l\sigma}(E)$: while finite as $\mu_\sigma \to 0+$ for $m = 1$ (which is why $\langle\Delta_\sigma\rangle$ in eq. 99 remains finite), all higher moments $m \geq 2$ of the LDoS diverge; hence so too does the variance $\langle(\delta\Delta_{V\sigma})^2\rangle$ (eq. 101a) and all higher moments of the distribution of Δ_σ. In otherwords all hell breaks loose as the transition is approached from the extended side, and once again the average value of Δ_σ is not remotely representative of its distribution. While fluctuations will dominate the critical regime close to the transition, our characterization of $f_\sigma(\Delta_\sigma)$ is of course just in terms of a most probable (or 'typical') value, which vanishes in a mean-field like fashion as the transition is approached. Simple though that undoubtedly is, it is nonetheless infinitely more meaningful than any focus on the mean value $\langle\Delta_\sigma\rangle$.

Time now to turn to the regime of localized states. Here we are in fact on our firmest ground, because we can determine explicitly an approximate functional form for the $f_\sigma(\Delta_\sigma)$ ($\equiv f_\sigma(\Delta_{j\sigma};\epsilon_{j\sigma})$), and can thus carry through the procedure of determining $\Delta_{\mathrm{mp};\sigma}$ as a function of the $\{\mu_\sigma\}$; leading to an effective stability analysis for the self-consistent existence of localized states, the breakdown of which signals the onset of the transition to extended states.

V. LOCALIZED STATES

Here were are interested in $\mu_\sigma \to 0+$ (for both σ), for which eqs. 91 reduce to:

$$\hat{f}_{V\sigma}(k;\epsilon_{j\sigma}) \overset{\mu_\sigma\to 0}{\sim} \left[1 + \int dV \int dx\; g_\sigma(V) M_\sigma(x;E;\epsilon_{j\sigma}) \left(\exp\left[\frac{ik\;|V|^2\mu_\sigma}{x^2}\right] - 1\right)\right]^K \tag{104a}$$

$$\hat{f}_{t\sigma}(k;\epsilon_{j\sigma}) \overset{\mu_{-\sigma}\to 0}{\sim} \left[1 + \int d\tilde{\xi} \int dx\; f_{0-\sigma}(E - \epsilon_{j\sigma} - \tilde{\xi} + x; \epsilon_{j\sigma} + \tilde{\xi})\tilde{P}(\tilde{\xi}) \left(\exp\left[\frac{ik\;|t(\epsilon_{j\sigma};\tilde{\xi})|^2\mu_{-\sigma}}{x^2}\right] - 1\right)\right]^{K_t} \tag{104b}$$

We begin by considering what the general structure of these equations imply.

First recall an elementary fact: if $f(x)$ is the normalized probability distribution for x, and $\tilde{f}(y)$ the distribution for $y = x/\phi$ (with ϕ a real constant), then the two are related by

$$f(x) \;=\; \frac{1}{|\phi|}\tilde{f}\Big(\frac{x}{\phi}\Big)$$

(such that$\int dx f(x) = 1 = \int dy \tilde{f}(y)$); or, equivalently, their Fourier transforms are related by $\hat{f}(k) = \hat{\tilde{f}}(\phi k)$. Note next from eq. 104 that $\hat{f}_{V\sigma}(k)$ and $\hat{f}_{t\sigma}(k)$ are functions *solely* of $\mu_\sigma k$ and $\mu_{-\sigma}k$ respectively. From the inverse FT eq. 71b, $f_{V\sigma}(\Delta_\sigma)$ and $f_{t\sigma}(\Delta_\sigma)$ are thus given by

$$f_{V\sigma}(\Delta_\sigma) \;=\; \frac{1}{\mu_\sigma}\tilde{f}_{V\sigma}\Big(\frac{\Delta_\sigma}{\mu_\sigma}\Big), \qquad f_{t\sigma}(\Delta_\sigma) \;=\; \frac{1}{\mu_{-\sigma}}\tilde{f}_{t\sigma}\Big(\frac{\Delta_\sigma}{\mu_{-\sigma}}\Big)\;. \tag{105}$$

$\tilde{f}_{\alpha\sigma}(y)$ ($\alpha = V, t$) must vanish as $y \to \infty$ (otherwise the distributions could not be normalized), whence all the weight in each $\tilde{f}_{\alpha\sigma}(y)$ is for *finite* Δ_σ/μ_σ (or $\Delta_\sigma/\mu_{-\sigma}$). In otherwords, since $\mu_\sigma \propto \eta \to 0+$ (for both σ), Δ_σ is proportional to $\eta \to 0+$ with probability unity for each constituent part of the distribution. The same is therefore true for the full distribution $f_\sigma(\Delta_\sigma)$, given by the convolution eq. 73b. This of course corresponds correctly to localized states.
[Note further that the above also shows why it would *not* be self-consistently possible to have e.g. $\mu_\sigma \propto \eta \to 0+$ but $\mu_{-\sigma}$ finite – in otherwords to have localized states in the σ-sector but extended states in the -σ-sector (a situation which obviously never arose in our original work). If such was conjectured, then all the weight in $f_{V\sigma}(\Delta_\sigma)$ would again be for finite Δ_σ/μ_σ (i.e. $\Delta_\sigma \propto \eta \to 0+$); but the distribution $f_{V\sigma}(\Delta_\sigma)$ would be for finite Δ_σ itself. Under the convolution eq. 73b, the latter would however ensure that the full $f_\sigma(\Delta_\sigma)$ had weight for finite Δ_σ. But

this corresponds to extended states, and as such is thus inconsistent with the starting assumption $\mu_\sigma \propto \eta \to 0+$. While this in essence is just an embodiment of the fact that localized and extended states cannot coexist at the same energy, it is reassuring to know that such an outcome should at least in principle be guaranteed by our approach.]

We now return to eqs. 104, to consider the leading $k \to 0$ behavior of $\hat{f}_{V\sigma}(k)$ and $\hat{f}_{t\sigma}(k)$. With the substitutions $u = x/[|k|\mu_\sigma |V|^2]^{1/2}$ and $u = x/[|k|\mu_{-\sigma}|t(\epsilon_{j\sigma};\tilde{\xi})|^2]^{1/2}$ in eqs. 104a,b respectively, we have

$$\begin{aligned}
\hat{f}_{V\sigma}(k;\epsilon_{j\sigma}) &= \left[1 + \sqrt{|k|\mu_\sigma}\int dV \int du\ |V| g_\sigma(V) M_\sigma(\sqrt{|k|\mu_\sigma}|V|u; E; \epsilon_{j\sigma})\ \left(\exp\left[\frac{i\ \mathrm{sgn}(k)}{u^2}\right] - 1\right)\right]^K \\
\hat{f}_{t\sigma}(k;\epsilon_{j\sigma}) &= \Big[1 + \sqrt{|k|\mu_{-\sigma}}\int d\tilde{\xi}\int du\ f_{0-\sigma}(E - \epsilon_{j\sigma} - \tilde{\xi} + \sqrt{|k|\mu_{-\sigma}}\ |t(\epsilon_{j\sigma};\tilde{\xi})|u; \epsilon_{j\sigma} + \tilde{\xi})\tilde{P}(\tilde{\xi})\ |t(\epsilon_{j\sigma};\tilde{\xi})| \\
&\qquad \times \left(\exp\left[\frac{i\ \mathrm{sgn}(k)}{u^2}\right] - 1\right)\Big]^{K_t}
\end{aligned}$$

and hence the leading low-k behavior

$$\begin{aligned}
\hat{f}_{V\sigma}(k;\epsilon_{j\sigma}) &\overset{k\to 0}{\sim} 1 + \sqrt{|k|\mu_\sigma}\ K \int dV \int du\ |V| g_\sigma(V) M_\sigma(0; E; \epsilon_{j\sigma})\ \left(\exp\left[\frac{i\ \mathrm{sgn}(k)}{u^2}\right] - 1\right) \\
\hat{f}_{t\sigma}(k;\epsilon_{j\sigma}) &\overset{k\to 0}{\sim} 1 + \sqrt{|k|\mu_{-\sigma}}\ K_t \int d\tilde{\xi}\int du\ f_{0-\sigma}(E - \epsilon_{j\sigma} - \tilde{\xi}; \epsilon_{j\sigma} + \tilde{\xi})\tilde{P}(\tilde{\xi})\ |t(\epsilon_{j\sigma};\tilde{\xi})|\ \left(\exp\left[\frac{i\ \mathrm{sgn}(k)}{u^2}\right] - 1\right) .
\end{aligned}$$

From eq. 83 ($D_{L\sigma}(E;\epsilon_{j\sigma}) = M_\sigma(x = 0; E; \epsilon_{j\sigma})$), and eqs. 90,89 for $\langle |t|\rangle$, together with

$$\int_{-\infty}^{\infty} du\ \left[\exp\left(\frac{i\ \mathrm{sgn}(k)}{u^2}\right) - 1\right] = -\sqrt{2\pi}\ [1 - i\ \mathrm{sgn}(k)] \tag{106}$$

(and recognising that $(1 - i\ \mathrm{sgn}(k))\sqrt{|k|} = (1 - i)\sqrt{k}$), we thus have

$$\hat{f}_{V\sigma}(k;\epsilon_{j\sigma}) \overset{k\to 0}{\sim} 1 - (1 - i)\sqrt{2\pi k\mu_\sigma}\ \ K\langle |V^{\sigma\sigma}|\rangle D_{L\sigma}(E;\epsilon_{j\sigma}) \tag{107a}$$

$$\hat{f}_{t\sigma}(k;\epsilon_{j\sigma}) \overset{k\to 0}{\sim} 1 - (1 - i)\sqrt{2\pi k\mu_{-\sigma}}\ \ K_t\langle |t|\rangle \tilde{D}_{L-\sigma}(E;\epsilon_{j\sigma}) \tag{107b}$$

(where $\langle |V^{\sigma\sigma}|\rangle = \int dV\ |V| g_\sigma(V)$). Hence from eq. 73 ($\hat{f}_\sigma(k;\epsilon_{j\sigma}) = \hat{f}_{V\sigma}(k;\epsilon_{j\sigma}) \times \hat{f}_{t\sigma}(k;\epsilon_{j\sigma})$),

$$\hat{f}_\sigma(k;\epsilon_{j\sigma}) \overset{k\to 0}{\sim} 1 - (1 - i)\sqrt{2\pi k}\left(\sqrt{\mu_\sigma}K\langle |V^{\sigma\sigma}|\rangle D_{L\sigma}(E;\epsilon_{j\sigma}) + \sqrt{\mu_{-\sigma}}K_t\langle |t|\rangle \tilde{D}_{L-\sigma}(E;\epsilon_{j\sigma})\right) . \tag{108}$$

The first, obvious point here is that the leading low-k behavior of the $\hat{f}_{\alpha\sigma}(k)$ (and hence $\hat{f}_\sigma(k)$) is $\hat{f}(k) - 1 \propto k^\gamma$ with $\gamma = \frac{1}{2}$. Coupled with the fact that the $\hat{f}_{\alpha\sigma}(k)$ depend on $\sqrt{k\mu_\sigma}$ (or $\sqrt{k\mu_{-\sigma}}$), this of course means that the distributions $\tilde{f}_{V\sigma}(\Delta_\sigma/\mu_\sigma)$ and $\tilde{f}_{t\sigma}(\Delta_\sigma/\mu_{-\sigma})$ (eq. 105) have a divergent average value (sec. IV B, eq. 93); indeed the asymptotic large $x = \Delta_\sigma/\mu_\sigma$ or $\Delta_\sigma/\mu_{-\sigma}$ behavior of the $\tilde{f}_{\alpha\sigma}(x)$ follows on general gounds as $\sim x^{-\gamma-1} = x^{-3/2}$ (which long tail is indicative of the divergent mean).

To obtain the distribution $f_\sigma(\Delta_\sigma)$ ($\equiv f_\sigma(\Delta_{j\sigma};\epsilon_{j\sigma})$) approximately, we proceed as in LW (eq. 26) and exponentiate eq. 108,[13,14]

$$\hat{f}_\sigma(k;\epsilon_{j\sigma}) \simeq \exp\Big(-(1 - i)\sqrt{2\pi k}\ \gamma_\sigma\Big) \tag{109a}$$

$$\gamma_\sigma = \sqrt{\mu_\sigma}K\langle |V^{\sigma\sigma}|\rangle D_{L\sigma}(E;\epsilon_{j\sigma}) + \sqrt{\mu_{-\sigma}}K_t\langle |t|\rangle \tilde{D}_{L-\sigma}(E;\epsilon_{j\sigma}) . \tag{109b}$$

Taking the inverse FT of this gives $f_\sigma(\Delta_\sigma) \simeq \gamma_\sigma\Delta_\sigma^{-3/2}\exp(-\pi\gamma_\sigma^2/\Delta_\sigma)$; or equivalently, for the distribution $\tilde{f}_\sigma(\tilde{\Delta}_\sigma)$ of $\tilde{\Delta}_\sigma = \Delta_\sigma/\eta$, given by $\tilde{f}_\sigma(\tilde{\Delta}_\sigma) = \eta f_\sigma(\Delta_\sigma)$ (*cf* eq. 105),

$$\tilde{f}_\sigma(\tilde{\Delta}_\sigma) = \tilde{\gamma}_\sigma\tilde{\Delta}_\sigma^{-3/2}\exp(-\pi\tilde{\gamma}_\sigma^2/\tilde{\Delta}_\sigma) \tag{110}$$

with $\tilde{\gamma}_\sigma = \gamma_\sigma/\sqrt{\eta}$. This is a Holtsmark-Markoff distribution (see e.g. §III of PWA, Phys. Rev. **109**, 1492 (1958)); which for $\tilde{\Delta}_\sigma \gg 1$ gives $\tilde{f}_\sigma(\tilde{\Delta}_\sigma) \propto \tilde{\Delta}_\sigma^{-3/2}$ (as indeed noted above). Its most probable value, denoted

$$y_\sigma := \tilde{\Delta}_{\mathrm{mp};\sigma} = \frac{\Delta_{\mathrm{mp};\sigma}}{\eta} , \tag{111}$$

follows trivially as $\tilde{\Delta}_{\mathrm{mp};\sigma} = 2\pi\tilde{\gamma}_\sigma^2/3$; and hence from eq. 109b we have

$$y_\sigma \;=\; \frac{\Delta_{\mathrm{mp};\sigma}(E;\epsilon_{j\sigma})}{\eta} \;=\; \left[\sqrt{\frac{\mu_\sigma}{\eta}}\; T_\sigma(E;\epsilon_{j\sigma}) \;+\; \sqrt{\frac{\mu_{-\sigma}}{\eta}}\; \tilde{T}_{-\sigma}(E;\epsilon_{j\sigma})\right]^2 \tag{112}$$

where

$$T_\sigma(E;\epsilon_{j\sigma}) \;=\; \sqrt{\tfrac{2\pi}{3}} K\langle|V^{\sigma\sigma}|\rangle D_{L\sigma}(E;\epsilon_{j\sigma}), \qquad \tilde{T}_{-\sigma}(E;\epsilon_{j\sigma}) \;=\; \sqrt{\tfrac{2\pi}{3}} K_t\langle|t|\rangle \tilde{D}_{L-\sigma}(E;\epsilon_{j\sigma})\;. \tag{113}$$

Since $\mu_\sigma = \eta + \Delta_{\mathrm{mp};\sigma}(E;\epsilon_{j\sigma})$ (eq. 64), eq. 112 is of course the desired pair of self-consistency equations which determine $y_\sigma = \Delta_{\mathrm{mp};\sigma}/\eta \geq 0$ in the localized regime,

$$\sqrt{y_\sigma} \;=\; \sqrt{1+y_\sigma}\; T_\sigma(E;\epsilon_{j\sigma}) \;+\; \sqrt{1+y_{-\sigma}}\; \tilde{T}_{-\sigma}(E;\epsilon_{j\sigma}) \qquad :\ \sigma = \uparrow/\downarrow\ ; \tag{114}$$

and the limits of stability of solutions to which determine the onset of the transition to extended states. This we now consider.

A. Transition Criterion

Consider then eq. 114 (dropping the arguments of T_σ and $\tilde{T}_{-\sigma}$ for clarity). Note first that, for $t_{jk}^{\sigma-\sigma} = 0$ (i.e. no electron tunneling), the $\tilde{T}_\sigma$ vanish and eq. 114 gives

$$\frac{\Delta_{\mathrm{mp};\sigma}}{\eta} \;=\; \frac{T_\sigma^2}{1-T_\sigma^2} \qquad :\ t_{jk}^{\sigma-\sigma} = 0\ . \tag{115}$$

This requires $T_\sigma^2 < 1$ for the stability of localized states; i.e. $T_\sigma < 1$, since the T_σ (and $\tilde{T}_\sigma$) are necessarily non-negative (eq. 113). Eq. 115 is precisely eq. 37 of LW;[15] and gives the familiar LW transition criterion of $T_\sigma^2 = 1$, i.e. (eq. 113) $\frac{2\pi}{3}[K\langle|V^{\sigma\sigma}|\rangle D_{L\sigma}(E;\epsilon_{j\sigma})]^2 = 1$. Notice trivially that, since the $\sigma = \uparrow/\downarrow$ sectors are decoupled and $T_\uparrow \neq T_\downarrow$ in general, nothing precludes the existence of localized states of energy E in one sector but extended states (of the same E) in the other.

We turn now to the general case where $\tilde{T}_\uparrow > 0$, $\tilde{T}_\downarrow > 0$ (physically, if one is non-vanishing then so too will be the other). Eqs. 114 for $y_\uparrow, y_\downarrow$ depend upon all four of $T_\uparrow, T_\downarrow, \tilde{T}_\uparrow, \tilde{T}_\downarrow$, and in the general case are quite subtle. We analyze them in Appendix **??**, from which the following key results arise. First, the transition to extended states for any given energy E occurs simultaneously in both σ-sectors/channels; i.e. $y_\uparrow = \Delta_{\mathrm{mp};\uparrow}/\eta$ and $y_\downarrow = \Delta_{\mathrm{mp};\downarrow}/\eta$ diverge simultaneously, which with non-zero coupling between channels is of course spot-on physically. The condition for the transition is given very simply by

$$1 \;=\; \frac{\tilde{T}_\uparrow\tilde{T}_\downarrow}{(1-T_\uparrow)(1-T_\downarrow)} \qquad :\ \text{transition} \tag{116}$$

as considered further below; with localized states arising for all $C := \tilde{T}_\uparrow\tilde{T}_\downarrow/[(1-T_\uparrow)(1-T_\downarrow)] < 1$ (with $T_\sigma < 1$ required). As the transition is approached, and both $y_\sigma \to \infty$, the y_σ are given by

$$\frac{\Delta_{\mathrm{mp};\sigma}}{\eta} \;=\; y_\sigma \;\sim \mathcal{A}_\sigma \left(1 \;-\; \tfrac{\tilde{T}_\sigma\tilde{T}_{-\sigma}}{(1-T_\sigma)(1-T_{-\sigma})}\right)^{-1} \tag{117a}$$

$$\mathcal{A}_\sigma \;=\; \frac{(1+\frac{\tilde{T}_{-\sigma}}{\tilde{T}_\sigma})}{2(1-T_\sigma)}\ , \tag{117b}$$

diverging with a common exponent of -1 as $C \to 1-$; but with finite σ-dependent amplitudes $\mathcal{A}_\sigma$ such that the ratio $y_\sigma/y_{-\sigma}$ remains finite as the transition is approached,

$$\sqrt{\frac{\Delta_{\mathrm{mp};\sigma}}{\Delta_{\mathrm{mp};-\sigma}}} \;=\; \sqrt{\frac{y_\sigma}{y_{-\sigma}}} \;=\; \frac{\tilde{T}_{-\sigma}}{(1-T_\sigma)} \;=\; \frac{(1-T_{-\sigma})}{\tilde{T}_\sigma} \qquad \text{transition.} \tag{118}$$

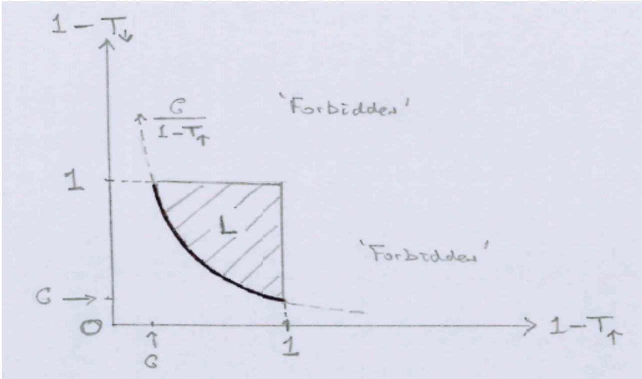

FIG. 1: Localized states in the $[1-T_\uparrow, 1-T_\downarrow]$-plane occur in the region ('L') bounded by the transition line $(1-T_\downarrow) = \mathcal{C}/(1-T_\uparrow)$ (thick line), $(1-T_\uparrow) = 1$ and $(1-T_\downarrow) = 1$. See text for discussion.

Now let's unpack this a little further. From the above, localized states occur for

$$(1-T_\downarrow) \;\geq\; \frac{\mathcal{C}}{(1-T_\uparrow)} \qquad : \; \mathcal{C} := \tilde{T}_\uparrow \tilde{T}_\downarrow \; > 0 \tag{119}$$

(with $0 \leq T_\sigma < 1$), where the equality corresponds to the transition itself. This is sketched in Fig. 1, with $(1-T_\uparrow)$ as the x-axis and $(1-T_\downarrow)$ as the y-axis. The combined regions $(1-T_\downarrow) > 1$ and $(1-T_\uparrow) > 1$ are of course 'forbidden', since $T_\sigma \geq 0$ necessarily. For $\mathcal{C} = \tilde{T}_\uparrow \tilde{T}_\downarrow = 0$ – no electron tunneling – localized states in both channels occur (as above) throughout the obvious positive square region bounded by $(1-T_\uparrow) = 1$, $(1-T_\downarrow) = 1$ and $(1-T_\uparrow) = 0$, $(1-T_\downarrow) = 0$. For some non-zero $\mathcal{C} \in (0,1)$, the phase boundary $(1-T_\downarrow) = \mathcal{C}/(1-T_\uparrow)$ is indicated in Fig. 1; along with the resultant region (hatched) of localized states, bounded by $(1-T_\downarrow) = \mathcal{C}/(1-T_\uparrow)$, $(1-T_\uparrow) = 1$ and $(1-T_\downarrow) = 1$.

In physical terms we can think of this as follows. Consider first the uncoupled case of no electron tunneling, $\mathcal{C} = 0$, for any fixed $T_\uparrow, T_\downarrow$ inside the positive square region of Fig. 1 (i.e. both $T_\sigma < 1$). The states of energy E are then localized in both wells/channels. Now switch on a small tunneling $\mathcal{C} = \tilde{T}_\uparrow \tilde{T}_\downarrow$. The states initially remain localized, but at a critical $\mathcal{C}_{\text{crit}} = (1-T_\uparrow)(1-T_\downarrow)$ the transition occurs and states delocalize simultaneously in both channels. This I think is a lovely example of many-body (de)localization: originally localized vibrational states can become delocalized (in Fock space) by switching on a sufficiently strong electron tunneling. Moreover, since the latter may itself originate from electron interactions – as mentioned at the beginning of sec. I – it is in this case electron interactions that induce delocalization.

A complementary way of thinking is to consider a fixed electron tunneling contribution $\mathcal{C} > 0$, and some initially chosen $T_\uparrow, T_\downarrow$ inside the hatched region of Fig. 1, such that states of energy E are localized. But on increasing $T_\uparrow$ and $T_\downarrow$ (along any 'trajectory' in Fig. 1), the phase boundary line will eventually be crossed and the states delocalize. The many-body delocalization in this case is induced by ramping up interactions between vibrational modes, reflected in increasing the T_σ (e.g. by increasing the anharmonic interactions embodied in $\langle |V^{\sigma\sigma}|\rangle$, eq. 113).

Finally, we mention a special case of the above, where $T_\sigma \equiv T$ and $\tilde{T}_\sigma \equiv \tilde{T}$ are independent of σ (corresponding in Fig. 1 to the diagonal line $(1-T_\downarrow) = (1-T_\uparrow)$). This pertains to the situation – certainly physically relevant – where the anharmonic interactions occurring in the two channels/wells are the same, so that the distributions $g_\sigma(V) \equiv g(V)$, $P_\sigma(\xi) \equiv P(\xi)$ are σ-independent. In that case, $y_\sigma = \Delta_{\text{mp};\sigma}/\eta$ is clearly σ-independent, i.e. $y_\sigma \equiv y = \Delta_{\text{mp}}/\eta$; and the solution to eq. 114 is trivially

$$\frac{\Delta_{\text{mp}}}{\eta} \;=\; \frac{[T+\tilde{T}]^2}{1-[T+\tilde{T}]^2}, \tag{120}$$

with the transition criterion now simply $T + \tilde{T} = 1$. Note that eq. 120 holds for all $T, \tilde{T}$ in the localized regime $T + \tilde{T} \leq 1$, i.e. not only close to the transition $T + \tilde{T} \simeq 1$ (for which eq. 120 reduces to $\Delta_{\text{mp}}/\eta \sim (2[1-(T+\tilde{T})])^{-1}$, in agreement with the general result eq. 117 for that instance).

Having now looked at the stability and breakdown of localized states, we return now to the regime of extended states, and the question of how to construct a suitable Padé approximant to interpolate in a mean-field like fashion between the two regimes.

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[1] In the model as it stands, note that only the 0-mode is taken to couple to the electron degree of freedom. If we also allowed the α-modes of H_{LW} to couple thus – via a term $H'' = \boldsymbol{\sigma}_z \sum_\alpha \lambda_\alpha (b_\alpha^\dagger + b_\alpha)$ – but neglected the anharmonic couplings $\phi_{0\beta\gamma}$ and $\phi_{\alpha\beta\gamma}$, then the model reduces to a conventional spin-boson model (see e.g. Leggett *et al*, Rev. Mod. Phys. **59**, 1, (1987)).

[2] Notice incidentally that $|\alpha, n\rangle = D(\alpha)|\alpha, n\rangle = e^{\alpha(b^\dagger - b)}|n\rangle$ gives $\frac{\partial}{\partial\alpha}|\alpha, n\rangle = (b^\dagger - b)e^{\alpha(b^\dagger - b)}|n\rangle = (b^\dagger - b)|\alpha, n\rangle$, whence $\frac{\partial}{\partial\alpha} \equiv (b^\dagger - b)$. Equivalently, $\frac{\partial}{\partial\alpha}|\alpha, n\rangle = ([b^\dagger - \alpha] - [b - \alpha])|\alpha, n\rangle = \sqrt{n+1}|\alpha, n+1\rangle - \sqrt{n}|\alpha, n-1\rangle$ (using eq. 27b and its counterpart for the destruction operator); whence for the ground state in particular, $\frac{\partial}{\partial\alpha}|\alpha, 0\rangle \equiv (b^\dagger - \alpha)|\alpha, 0\rangle$ $(= |\alpha, 1\rangle)$.

[3] Or Bessel function of imaginary argument (which despite its name is well defined for real z).

[4] At least modulo any subtleties that might be associated with the large-n limit and classical correspondence.

[5] In practice we can take $\gg$ to mean $\gtrsim$ in the definition eq. 48 of the strong coupling regime.

[6] A minor initial comment (see also footnote [27] of LW). Strictly speaking in eq. 56, $S_{j\sigma}(E)$ refers to $S_{j\sigma}^{(i)}(E)$, meaning that the site $i\sigma$ before site $j\sigma$ is excluded (see fig. 1 of LW); likewise $S_{l\sigma}(E)$, $S_{k-\sigma}(E)$ refer strictly to $S_{l\sigma}^{(j)}(E)$, $S_{k-\sigma}^{(j)}(E)$, with site $j\sigma$ excluded. It is for this reason that e.g. the first term on the rhs of eq. 56 has K terms in the sum, rather than $K+1$. It is in fact the equations for $S_{j\sigma}^{(i)}(E)$ etc that are actually analyzed in eq. 56 *ff* (as indeed is required when we later take the distributions $F_\sigma(E_{n\sigma}, \Delta_{n\sigma})$ for the real and imaginary parts of the self-energy for site $n\sigma$ to be n-independent). By the same token, $G_{j\sigma}(E)$ in eq. 55 refers strictly to $G_{j\sigma}^{(i)}(E)$ (and this in practice is analyzed); but at the end of the day we then neglect the site-restriction and conflate $G_{j\sigma}^{(i)}(E) \equiv G_{j\sigma}^{(i)}(E)$ – this being immaterial in practice at our level of analysis (and an $\mathcal{O}(1/K)$ effect, with K the state-space connectivity).

[7] The lowest-order contributions neglected are third and fourth order RPS terms $\mathcal{O}(Vt^2)$, $\mathcal{O}(V^2t^2)$ and $\mathcal{O}(t^4)$.

[8] The obvious exception is when the electronic level detuning $\epsilon \simeq 0$.

[9] The distribution $f_\sigma(\Delta_{j\sigma}; \epsilon_{j\sigma})$ is of course non-zero only for $\Delta_{j\sigma} \geq 0$, since $\Delta_{j\sigma} \geq 0$ by analyticity.

[10] No u, how indulgent (!).

[11] For this reason, together with the fact that $f_\sigma(\Delta)$ is non-zero only for $\Delta > 0$, $\Delta_{\mathrm{mp};\sigma}$ and $\langle\Delta_\sigma\rangle$ will never strictly coincide.

[12] The finite mean here reflects occurrences which have a vanishingly small probability, but which nonetheless dominate the mean; as discussed e.g. in §VD pg 5007 of LW, re the 'renormalized' golden rule.

[13] Note that direct exponentiation of eq. 108, as here, is precisely the same as exponentiating eqs. 107 for $\hat{f}_{V\sigma}(k)$, $\hat{f}_{t\sigma}(k)$ separately, and then taking their product (eq. 73a) to give $\hat{f}_\sigma(k)$.

[14] I have a feeling this exponentiation underlies the Holtsmark-Markoff method (e.g. §III of PWA 1958). Need to stew on this.

[15] Note that what we here call T_σ^2 was called T in LW. The structure of eqs. 114 render our present definitions more natural, as seen below and in Appendix **??**.