Lecture 14: Many-fermion N-body Systems

We will be discussing a series of N-body techniques in QM in the next two weeks. Here N-body means that it is not an infinite system like the electron gas, but a finite one: an atom, a nucleus, perhaps even heavy quarks in a heavy baryon.

We will discuss many approaches to such problems. Here I would like to describe a method that is widely used in many fields and that is heavily numerical. It has the attractive feature that it maps onto our picture of many-body systems in second quantization in a very natural way. That why I want to discuss in now. The discussion also illustrates a few of the difficult aspects of many-fermion problems that sometimes obscured in other approaches.

Finite Fermi systems

Given a many-fermion Hamiltonian $\hat{H}$

$$\hat{H} = \sum_{\alpha,\beta} \langle \alpha | T | \beta \rangle a_\alpha^\dagger a_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma,$$

the task of solving the time-independent Schroedinger equation

$$\hat{H}|\Psi\rangle = E|\Psi\rangle$$

within a Hilbert space spanned by the basis states

$$|n_1 n_2 ... n_\infty\rangle$$

is equivalent to diagonalizing the matrix $\hat{H}$ within this basis. Then main difficulty is that the single-particle states from which the N-particle basis states are constructed are generally of infinite dimension, and consequently the many-body basis is certainly of infinite dimension. Thus the required diagonalization is not possible by any numerical means.

This forces one to truncate the basis to some finite number. There are two approaches to this truncation. One possibility is to evaluate the Hamiltonian without corrections in some P space. By the variational theorem we have previously discussed, this has the advantage of giving a ground-state energy that is a rigorous upper bound to the true energy: in the end, the ground state energy is simply the expectation of the H between a wave function. This approach may give very good results if the coupling to Q is weak.

Alternatively, one can introduce a H^{eff} that will yield a better ground state (or excited states) in P. This approach also has its limitations. First, we no longer have a variational estimate of the energy. Second, the calculation of H^{eff} by direct means through, say, the Bloch Horowitz equation is essentially equivalent to the origin problem solved in the full $P+Q$. But we have seen ways to finesse this problem, e.g., by using effective theory. Specifically we showed that if our P captures the correct long-range behavior of our problem, then we could introduce a series of short-range effective operators that act within P, correcting for the omissions in Q. The coefficients off these short-range operators can be determined from data.

Alternatively one can try to develop a theory for the missing short-range physics that allows one to correct for the effects of Q, without solving the full problem in Q. For example, in nuclear physics where the nuclear system is in some sense dilute yet the missing physics is characterized by very short range interactions, one might anticipate the the two-nucleon ladder diagrams (repeated rescattering of two nucleons at short range) might be an important part of the missing physics. This is called the Brueckner G-matrix.

In principle if we solve the Schroedinger equation with the exact H^{eff} (which is state dependent), we obtain the exact eigenvalue and restriction of the true wave function to P. In practice, since we approximate H^{eff}, neither of these results hold.

The Hamiltonian: Antisymmetry and the center-of mass

Finite Fermi systems some times present challenges connected with properly treating the center of mass. Generally we are interested in intrinsic excitations, in finite systems – the energy levels of molecules, electrons, or nuclei. For an atom, because the nucleus is heavy and thus can usually be treated as a static source, no difficulties arise: we can treat the nucleus as infinitely heavy, fix it is space, and describe the motion of the electrons relative to the nucleus in terms of Z coordinates $\vec{r}_i$. Antisymmetric Slater determinants are created as we have discussed, and we can represent these in terms of our second quantized occupation-number states.

But that description might not be appropriate in other situations like a nucleus, where the intrinsic motion is connected with the relative coordinates describing the motion of roughly equal-mass nucleon constituents. The potential term in the Hamiltonian

$$H = \sum_i^N \frac{\vec{p}_i^{\,2}}{2M} + \frac{1}{2}\sum_{i\neq j=1}^{N} V_{ij}$$

is translatiuonally invariant $V_{ij} = V(\vec{r}_i - \vec{r}_j)$. It depends on the proper 3(N-1) intrinsic coordinates: if one knows the 3(N-1) coordinates $\vec{r}_1 - \vec{r}_2$, $\vec{r}_1 - \vec{r}_3$,...,$\vec{r}_1 - \vec{r}_N$, then any $\vec{r}_i - \vec{r}_j$ can be expressed in terms of these coordinates. The kinetic energy appears to depend on $3N$ coordinates, but it can be factored into intrinsic and center-of-mass pieces

$$\begin{aligned}\sum_{i=1}^{N} \vec{p}_i^{\,2} = \frac{1}{2N} \sum_{i,j=1}^{N} (\vec{p}_i^{\,2} + \vec{p}_j^{\,2}) &= \frac{1}{2N} \sum_{i,j=1}^{N} \left[(\vec{p}_i - \vec{p}_j)^2 + 2\vec{p}_i \cdot \vec{p}_j \right] \\ &= \frac{1}{2N} \sum_{i \neq j=1}^{N} (\vec{p}_i - \vec{p}_j)^2 + \frac{1}{N} \left[\sum_{i=1}^{N} \vec{p}_i \right] \cdot \left[\sum_{j=1}^{N} \vec{p}_i \right] \end{aligned} \tag{1}$$

What this means is that our Hamiltonian above was really not written in an intelligent way. In should have been written

$$H = H_{\rm CM} + H_{\rm intrinsic}$$

$$H_{\rm CM} = \frac{1}{2m\,N} \vec{P}_{\rm CM}^{\,2} \quad \text{where} \quad \vec{P}_{\rm CM} = \sum_{i=1}^{N} \vec{p}_i$$

$$H_{\rm intrinsic} = \frac{1}{2m\,N} \sum_{i \neq j=1}^{N} (\vec{p}_i - \vec{p}_j)^2 + \frac{1}{2} \sum_{i \neq j=1}^{N} V_{ij} = \frac{1}{2} \sum_{i \neq j=1}^{N} (T_{ij} + V_{ij})$$

The center-of-mass (CM) Hamiltonian is trivial – the nucleus as a whole behaves plane wave for a particle of mass mN. But the remaining intrinsic Hamiltonian is now complicated. In analogy with the familiar treatment of two-body scattering, where the center-of-mass and relative wave functions are separated, with the latter depending on $\vec{r}_1 - \vec{r}_2$, one can introduce a complete set of intrinsic coordinates

$$\dot{\vec{r}} = \frac{1}{\sqrt{2}} [\vec{r}_1 - \vec{r}_2] \quad \dot{\vec{r}}_2 = \frac{1}{\sqrt{6}} [2\vec{r}_3 - (\vec{r}_1 + \vec{r}_2)] \;\; .... \;\; \dot{\vec{r}}_{N-1} = \frac{1}{\sqrt{(N-1)N}} [(N-1)\vec{r}_N - (\vec{r}_1 + ... + \vec{r}_{N-1})]$$

which, together with the CM coordinate $\vec{r}_{\rm CM} = (\vec{r}_1 + ...\vec{r}_N)\sqrt{N}$, are equivalent to the original coordinates $\vec{r}_1, ..., \vec{r}_N$. The $N-1$ Jacobi coordinates are an appropriate choice for describing the $H_{\rm intrinsic}$. In can be shown, for instance, that

$$\frac{1}{2m\,N} \sum_{i \neq j=1}^{N} (\vec{p}_i - \vec{p}_j)^2 = \frac{1}{2m} \sum_{i=1}^{N} \dot{\vec{p}}_i^{\,2} \quad \text{where} \quad \dot{\vec{p}}_i = \frac{\hbar}{i} \dot{\vec{\nabla}}_i$$

One might think that the division above is great because the hard part of the problem - the intrinsic motion - now involves three fewer degrees of freedom, and we have even managed to write the kinetic energy in a way that it appears to be "one-body.." But this is generally not so: one

important property of our 3N-degree-of-freedom basis – a direct product of single-particle bases – is that the antisymmetry was trivial. It becomes a much more difficult task (in almost all cases) to antisymmetrize wave functions written in Jacobi coordinates . This becomes exhausting for systems of ~ 10 or more particles.

This leaves one other possibility, solve the problem defined by $H_{\rm intrinsic}$ but do so in the overcomplete but easily antisymmertrized N-particle basis. As our Hamiltonian is explicitly independent of CM motion, one might think there is no harm – at most one would get the intrinsic ground state accompanied by some accompanying center-of-mass state. Intrinsic states where the center-of-mass is in different states would not fix. In the full Hilbert space, one would get a degenerate ground state – one intrinsic state accompanied by many possible center-of-mass states. One could trivially break that degeneracy by adding H_{CM} back in.

There is a flaw in this argument – almost any calculation one contemplates cannot be done in the full Hilbert space, and thus that space must her truncated into a finite number of states. Unfortunately, in almost all cases, this truncation destroys the ability to factor wave functions into CM and intrinsic components.

If we restrict ourselves to compact bases appropriate for describing bound states, there is one exception to this rule, the harmonic oscillator. If P is defined as all many-body states formed from HO single-particle states in which the total number of quanta in the Slater determinant is $\leq \Lambda$ (that is, the sums of all the principle HO quantum numbers N for the individual orbitals in a Slater determinant cannot exceed Λ), then this truncated basis of Slater determinants is *separable*:

$$\{\Psi(1,...,N)_\Lambda\} = \{|\Psi^\Delta_{\rm CM} \otimes \Psi^{\Lambda-\Delta}_{\rm intrinsic}, \Delta = 0, 1, ...\Lambda\}$$

In such a separable space, there will be a set of intrinsic states accompanied by the HO CM ground state (1s state); there will be a second set that are accompanied by the the HO CM first excited state (1p state); a third set ... These sets will not interact with one another because $H_{\rm intrinsic}$ cannot mix states whose CMs are in different states. Thus by adding the HO CM Hamiltonian to $H_{\rm intrinsic}$, one will obtain a non degenerate ground state consisting of the desire intrinsic state times a center-of-mass wave function in the 1s state. Then one can subtract the 3/2 $\hbar omega$ associated with the CM motion to obtain the intrinsic energy.

Much more could be said ... but the bottom line is that there are a number of subtle issues to keep in mind.

Many fermion problems vs the computer Regardless of the approach taken to address the mixing physics in Q, we will assume that an approximate H^{eff} has been identified – or that the coupling of Q to P is sufficiently weak that we can use the bare H. How are many-fermion calculations actually none? We will find out there are many approaches, but let me describe here the direct numerical approach, because its makes such good use of the formulation in second quantization.

Suppose we have N particle and a Hilbert space spanned by m distinct single-particle states, $1....m, m \geq N$. Then the state vectors in second quantization are

$$a^\dagger_{i_N}...a^\dagger_{i_2}a^\dagger_{i_1}|0\rangle \text{ where } \; i_N... > i_2 > i_1$$

If we map our single-particle states onto one or more computer words, depending on the size of m, we cant represent this state vector as a string of 1s (occupied single-particle states) and 0s (unoccupied). If N=4 and m=10

$$a^\dagger_9 a^\dagger_7 a^\dagger_4 a^\dagger_2|0\rangle \rightarrow \text{orbitals}: \quad \begin{array}{cccccccccc} 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 \end{array}$$

The Hilbert space would include all such computer words based on ten bits, four occupied, subject to ancillary constraints. (For example, in the HO, we might keep only those configurations where the sum over single-particle quantum are less than some Λ, to create a more limited but separable Hilbert space.) To do quantum mechanics we need to calculate matrix elements. We have both one-body and two-body operators generally (and some times more complicated operators. Let's consider the two-body case. Then

$$\langle\phi_i| \; \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V|\delta\gamma\rangle a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta \; |\phi_j\rangle = \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V|\delta\gamma\rangle \;\; \langle\phi_i^{\beta\alpha}|\phi_j^{\gamma\delta}\rangle$$

$$\text{where } \; |\phi_j^{\gamma\delta}\rangle = a_\gamma a_\delta \; |\phi_j\rangle \qquad |\phi_i^{\beta\alpha}\rangle = a_\beta a_\alpha \; |\phi_i\rangle$$

Noting that

$$\begin{aligned} \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|V|\delta\gamma\rangle a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta &= \frac{1}{2}\sum_{\beta>\alpha \;\; \gamma>\delta}\langle\alpha\beta|V|\delta\gamma\rangle \; a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta + \frac{1}{2}\sum_{\alpha>\beta \;\; \gamma>\delta}\langle\alpha\beta|V|\delta\gamma\rangle \; a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta \\ &+ \frac{1}{2}\sum_{\beta>\alpha \;\; \delta>\gamma}\langle\alpha\beta|V|\delta\gamma\rangle \; a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta + \frac{1}{2}\sum_{\alpha>\beta \;\; \delta>\gamma}\langle\alpha\beta|V|\delta\gamma\rangle \; a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta \end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{2}\sum_{\beta>\alpha}\sum_{\gamma>\delta}\langle\alpha\beta|V|\delta\gamma\rangle\ a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta - \frac{1}{2}\sum_{\beta>\alpha}\sum_{\gamma>\delta}\langle\beta\alpha|V|\delta\gamma\rangle\ a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta \\
&- \frac{1}{2}\sum_{\beta>\alpha}\sum_{\gamma>\delta}\langle\alpha\beta|V|\gamma\delta\rangle\ a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta + \frac{1}{2}\sum_{\beta>\alpha}\sum_{\gamma>\delta}\langle\beta\alpha|V|\gamma\delta\rangle\ a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta \\
&= \frac{1}{2}\sum_{\beta>\alpha}\sum_{\gamma>\delta}\langle\alpha\beta-\beta\alpha|V|\delta\gamma-\gamma\delta\rangle\ a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta
\end{aligned}
$$

our expression becomes

$$
\frac{1}{2}\sum_{\beta>\alpha}\sum_{\gamma>\delta}\langle\alpha\beta-\beta\alpha|V|\delta\gamma-\gamma\delta\rangle\ \ \langle\phi_i^{\beta\alpha}|\phi_j^{\gamma\delta}\rangle
$$

$$
\text{where}\ \ |\phi_j^{\gamma\delta}\rangle = a_\gamma a_\delta\ |\phi_j\rangle \qquad |\phi_i^{\beta\alpha}\rangle = a_\beta a_\alpha\ |\phi_i\rangle
$$

So we need only calculate for all $\beta < \alpha$ and state vectors i

$$
a_\beta a_\alpha\ |\phi_i\rangle = \begin{cases} 0 & \text{if } \alpha \text{ or } \beta \text{ is unoccupied in } i \\ (-1)^{S_\beta+S_\alpha}|\phi_i^{\tilde{\beta}\tilde{\alpha}}\rangle & \text{otherwise} \end{cases}
$$

Now $S_\beta + S_\alpha = (n_\infty + ... + .n_{\alpha-1}) + (n_\infty + ... + n_{\beta-1}) = n_\beta + n_{\beta+1} + ...n_{\alpha-1}$ These operations and the fermion phase can be calculated very rapidly using bit compares. For two-particle annihilation

1. Take

$$
|\phi\rangle = a^\dagger_9 a^\dagger_7 a^\dagger_4 a^\dagger_2|0\rangle \rightarrow \text{orbitals}: \quad \begin{array}{cccccccccc} 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ 0 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 \end{array}
$$

   Suppose we want $a_2|\phi\rangle$, and we do not know whether the 2nd slot is occupied. Then take 1, do a bit shift to form $|I_2\rangle \equiv 0000000010$. Form $J_2 = (|\phi\rangle\ AND\ I_2)$. If $J_2 = I_2$ the orbit was occupied. Then $a_2|\phi\rangle = |\phi\rangle - I_2$ (up to a sign).

2. Repeat to get $a_7 a_2|\phi\rangle = 0 \quad 1 \quad 0 \quad 0 \quad 0 \quad 0 \quad 1 \quad 0 \quad 0 \quad 0$ (up to a phase).

3. The phase, but our discussion above is 1+(number of bits between locations 7 and 2). So form

$$
\begin{aligned}
I_{7,2} = I_7 - I_2 &= 1000000 \\
&- \quad\ 10 = 111110
\end{aligned}
\tag{2}
$$

Then $(a_7 a_2|\phi\rangle \ AND \ I_{7,2}) = 0000001000$. Count the bits (machines have instructions to do this) and add one for the phase.

This example gives you the flavor of how second quantized many-body states might be efficiently stored on a computer, then acted on to form state vectors, using fast internal instructions for bit compares and bit counting.

Diagonalization: the Lanczos Algorithm

One can envision that the above algorithm might give you a massive Hamiltonian. In the end, a solution of the time-independent Schroedinger equation will be required

$$H|\Psi\rangle = E|\Psi\rangle$$

within this massive number Hilbert space. How is this done. Well, if one uses standard Householder methods, the time required would scale by n^3, where n is the dimension of the matrix. Thus if one's computer takes 1 second to diagonalize a 100 $\times$ 100 matrix, is would take 10^{21} seconds to diagonalize a $10^9 by 10^9$ one. That is not going to work.

There is a lovely algorithm that I think of as linear algebra's perfect effective theory, that allows one to overcome some difficulties. This algorithm can be adapted to solve three problems:

- To find the extremum eigenvalues and eigenvectors – the smallest and largest – of a very large matrix, recursively. Thus one can the ground state, the gap to the first excited states, and perhaps a dozen more low-lying states efficiently, in this way.

- To determine inclusive response functions. Often after solving for the ground state, the QM application will ask one to operate on the ground state and sum the response to all possible final states. The Lanczos algorithm provides an elegant solution to this problem.

- One has the ground state or an excited state, but needs the vector produced when the Green's function $1/E - H$ operates on the ground state. Again, the Lanczos algorithm can efficiently find that vector.

I will discuss only the first application here.

The algorithm is quite simple. Let H be a Hermitian operator, and let $|v_1\rangle$ be any vector in the N-dimensional Hilbert space in which H operates, normalized so that $\langle v_1|v_1\rangle = 1$. We recursively

form a basis in which we can represent H

$$\begin{aligned} 1)\ H|v_1\rangle &= \alpha_1|v_1\rangle + \beta_1|v_2\rangle \\ 2)\ H|v_2\rangle &= \beta_1|v_1\rangle + \alpha_2|v_2\rangle + \beta_2|v_3\rangle \\ 3)\ H|v_3\rangle &= \beta_2|v_2\rangle + \alpha_3|v_3\rangle + \beta_3|v_4\rangle \\ &..... \end{aligned}$$

In the first step α_1 and β_1 are found from $\alpha_1 = \langle v_1|H|v_1\rangle$ and $\beta_1|v_2\rangle = (H-\alpha)|v_1\rangle$. Each of the Lanczos vectors $|v_i\rangle$ is normalized. The algorithm mathematically guarantees that every new $|v_i\rangle$ is orthogonal to all previous vectors. Numerically, small nonorthogonalities grow, so most implementations "re-orthogonalize" each new vector to all previous vectors. If carried out to completion, on the Nth step one would have

$$H|v_N\rangle = \beta_{N-1}|v_{N-1}\rangle + \alpha_N|v_N\rangle + \beta_N|v_{N+1}\rangle$$

with $\beta_N \equiv 0$. The Hilbert space is only N-dimensional, so the algorithm would necessarily truncate at this point.

In practice the algorithm is truncated at $n \ll N$ steps, yielding the triadiagonal matrix

$$H \to H^{eff} = \begin{pmatrix} \alpha_1 & \beta_1 & 0 & 0 & \dots & \\ \beta_1 & \alpha_2 & \beta_2 & 0 & \dots & \\ 0 & \beta_2 & \alpha_3 & \beta_3 & ... & \\ 0 & 0 & \beta_3 & \alpha_4 & \dots & \\ \vdots & \vdots & \vdots & \vdots & & \beta_{n-1} \\ & & & & \beta_{n-1} & \alpha_n \end{pmatrix}$$

This algorithm has a remarkable property. After n iterations, the Lanczos matrix contains $2n-1$ constants. These constants contain precisely the same informations as:

$$\{\alpha_1, ..., \alpha_n;\ \beta_1, ..., \beta_{n-1}\} \ \leftrightarrow \{\langle v_1|H^k|v_1\rangle,\ k = 1, ..., 2n-1\}$$

One can see this by going back to the first few steps of the algorithm. Note

$$\langle v_1|H|v_1\rangle = \alpha_1$$

$$\langle v_1|H^2|v_1\rangle = (\langle v_1|\alpha_1^* + \langle v_2|\beta_1^*)(\alpha_1|v_1\rangle + \beta_1|v_2\rangle) = |\alpha_1|^2 + |\beta_1|^2$$

$$\begin{aligned}\langle v_1|H^3|v_1\rangle &= (\langle v_1|\alpha_1^* + \langle v_2|\beta_1^*)H(\alpha_1|v_1\rangle + \beta_1|v_2\rangle) \\ &= (\langle v_1|\alpha_1^* + \langle v_2|\beta_1^*)(\alpha_1^2|v_1\rangle + \alpha_1\beta_1|v_2\rangle + \beta_1^2|v_1\rangle + \beta_1\alpha_2|v_2\rangle + \beta_1\beta_2|v_3\rangle) \\ &= \alpha_1^*(\alpha_1^2 + \beta_1^2) + |\beta_1|^2(\alpha_1 + \alpha_2)\end{aligned}$$

It it interesting to think of this as a distribution. One picks some arbitrary $|v_1\rangle$. If $|\Psi_{E_i}\rangle$ are the exact eigenfunction of the full matrix H, then we can write

$$|v_1\rangle = \sum_{i=1}^{N} a_i|\Psi_{E_i}\rangle \;\text{ with }\; \langle v_i|v_1\rangle = \sum_{i=1}^{N}|a_i|^2 = 1$$

Now the $|a_i|^2$ define a distribution in energy - N points and weights, with the weights being the probability of $|v_1\rangle$ in eigenstate i

$$D(E) = \sum_{i=1}^{N}|a_i|^2\delta(E - E_i)$$

and

$$\langle v_1|H^k|v_1\rangle = \sum_{i=1}^{N}|a_i|^2E_i^k = \int dE D(E)E^k$$

That is, the full H defines a distribution of N points and N weights, subject to the constraint that the zeroth moment is 1 by normalization. Thus there are $2N-1$ independent pieces of information. But we can also diagonalize the Lanczos matrix. Let those eigenfunctions be denoted $|\Psi_{\epsilon_i}^L\rangle$. Then

$$|v_1\rangle = \sum_{i=1}^{n} b_i|\Psi_{\epsilon_i}^L\rangle \;\Rightarrow D^L(E) = \sum_{i=1}^{n}|b_i|^2\delta(E - \epsilon_i)$$

In can be shown that $D(E)$ and $D^L(E)$ have identical moments for $H^k, k = 1, ..., 2n-1$. Thus the Lanczos algorithm provides a numerically stable solution to the classical moments problem, the representation of a distribution by points and weights that exactly preserves the moments. The Lanczos algorithm systematically and recursively extracts the long-wavelength moments information from the true distribution. This explains why I term the Lanczos algorithm a numerical effective theory.

This qualitatively explains how the Lanczos algorithm can do so much:

- Extremum eigenstates: The lowest and highest eigenvalues are generally somewhat set off from the bulk of the spectrum – spectral distributions tend to have the highest density in the center – thus these extremum eigenvalues have exception weight in high lying moments. So

when $n \sim 100$ and the 200th moment is being captured, the distribution in n must have a weight at the true eigenvalue, e.g., $\epsilon_1 \to E_1$. Typically perhaps 5-10 of the lowest states may converge by $n \sim 100$.

- Response functions. One can use the algorithm to calculate a ground state $|g.s\rangle$, operate on the ground state by an operator $\hat{O}$, then select

$$|v_1\rangle = \frac{\hat{O}|g.s.\rangle}{\sqrt{\langle g.s.|\hat{O}^\dagger \hat{O}|g.s.\rangle}}$$

  and thereby determine the distribution of the response over the full eigenspectrum. One can see that the algorithm should allow one to evaluate inclusive response functions.

- In calculating Green's functions, one could envision inverting H^{eff} to estimate that Green's function. In fact, there is a representation for $G(E)|v_1\rangle$ in terms of a sum over the Lanczos vectors, where the coefficients are continued fractions that depend on the αs, βs, and E, and where these coefficients are updated with every iteration. The Lanczos Green's function algorithm is often rapidly converging.

I took this detour to discuss numerical QM because young people interested in either theoretical or experimental physics are likely to see leadership-class computing become an increasing important tool for the field. Over the last decade machines have progressed from the terascale to the 20 petascale level. The power of available machines 20 years hence is almost unimaginable. Berkeley Physics is involved in the Designated Emphasis in Computational Science and Engineering program that allows graduate students to gain experience in advanced computing during thesis work.