

ask about

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## 880.05 Class #1

### Handouts:

- print outs of 880.05 home page (references) and info page
  - phenomenological potentials + phenomenological/QCD V slides
  - dot's, S. Weinberg quote on RG slides
  - Three-nucleon force background slides
  - Digital potentials, resolution analogy slides
  - First 4 pages of "Effective Field Theory at Finite Density Systems"
  - First 4 pages of Blume/Daily SVM calculation of 4 fermion system
  - FCI basis size scaling slides
- [b, c, d, e, h were handed out together]

### Course logistics

• Step through info sheet

• "Many-Body Physics: EFT, RG, and Computation"

• no text required but you may decide one or more of the recommended references are worth having

(warning: many are expensive, although Dover editions when old)

In place of a text, we will reference excerpts from various texts (either linked or handed out) and I will post handwritten class notes in pdf format on the web page.

⇒ Password protected ⇒ username: physics password: 880.05

• We'll have nuclear examples in mind and focus on methods useful for nuclear problems, but the course material is more general. Nuclear many-body problems have complications and we always "do the easy problems first".

• Also we will deal with current, unsolved problems (at least in part)

⇒ learn tools to solve them

• Methods: path integrals and effective actions, effective field theory (EFT), renormalization group (RG).

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you already know some important many-body physics! ②

Sounds scary but...

Prerequisites are quantum mechanics and statistical mechanics 1st year courses, and knowledge of linear algebra, etc. matrices

- Field Theory is not assumed, but we will use it!
- Your job is to ask many questions if I assume too much.
- How is this possible? A big help is thinking about implementation of many-body techniques on computers.

concentrate on operational instead of formal details

- practical  $\Rightarrow$  you need to actually calculate eventually and the implementation details matter
- good way to learn methods or gain deeper understanding
- makes formal math much more accessible:  $\rightarrow$  infinite, continuous  $\rightarrow$  finite, discrete (e.g. in path integrals, reduce to manipulations of finite matrices, functional calculus  $\rightarrow$  ordinary calculus, etc.)

- People auditing are very welcome but note that pace is set by backgrounds of registered students.
- But please ask questions!
- We will stop regularly and ask you questions to discuss with neighbors  $\rightarrow$  feedback on understanding and keeps you awake!

### Instructors:

Dick Furnstahl — research specialization is nuclear many-body theory using EFT, RG, DFT, CC, ... [Note: call me "Dick" if possible]

Joaquin Arut — postdoc in NTG, recent winner of Kimmel award for early achievement in many-body theory: Calculations of cold atoms (formal + numerical), graphene, orbital-based DFT. Application of lattice QCD methods to condensed matter problems.

\*Seminar Thursday morning in PRB 4138 11am "Lattice QCD Meets Condensed Matter Physics" All are invited to attend.

### Schedule:

- We'll take a break in the middle (extra questions or stretching or...)
- We'll schedule extra (optional) sessions for problems or special topics (e.g. chiral EFT or solving graphene)

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Office Hours

- dropping by PRB M2018 (Furnstahl) early or PRB M2064 (Dout) late will work a lot of the time (just interrupt!)
- Plus chocolate is freely available!
- or schedule in class or via email
- we'll figure out "official" times as we go
- ask about anything

Grading

- Only problem sets — <sup>with</sup> opportunity to self-correct
- You are strongly encouraged to collaborate except for last problem set
- Only goal is for everyone to maximize learning (so don't worry if you are overwhelmed at times)

Philosophy

- not enough time for thorough formal developments
- ⇒ more heuristic or jump in with computational version: operational
- build around illustrative examples (or analogies)
- In problem sets: extend, refine, treat analogous examples

Web Page (see handout with snapshot of home page)

- source of handouts, notes, problem sets, announcements
- background or supplementary reading assignments (available ahead of time)
  - note variational methods reading — more to come soon!
- note long list of recommended references
  - several are cheap ⇒ worth getting
- Also review articles (return to "EFT and Finite-Density Systems")

References:

- Step through some of the comments (have AHS and NHO available)
- Comment on FHW: my corrections; rigorous and correct and accessible, but many new methods (including all of our topics)

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## Overview of Course: The Big Picture

- We'll consider nonrelativistic many-body problems
  - goal: given forces (potentials) between 2 (or more) particles,  

$$[ \text{eg. } H = \sum_i T_i + \sum_{i,j} V_{ij} + \sum_{i,j,k} V_{ijk} + \dots ]$$
 calculate observables for a many-particle system
  - system could be atoms in a trap, nucleus, electron density in molecule, liquid helium, and so on. ← for  $pc \ll mc^2$  with explicit  $c$
  - nonrelativistic  $\Rightarrow$  momentum  $p \ll$  particle mass  $M$  (so  $v \ll c$ )
    - Where is this not valid? (eg. some aspects of heavy atoms)
    - for nuclei, relativistic covariance (scalar vs. time component of four-vector) is believed to be important. But nonrelativistic expansion should be ok (if possibly slowly converging for some features)
  - observables include ground state energy (and density distribution in finite systems), equation of state, other thermodynamic functions, details of phase transitions, energies and lifetimes of excited states, linear response to external probes...

These  
lead to  
utility of  
EFT  
and imply  
universality

- Sounds like condensed matter problems. What do Altland and Simons say? (in Chapter 1) about the basic principles in generic condensed matter systems:
  - ① Structural reducibility: We don't need to treat all components of the Hamiltonian simultaneously. Eg. Born-Oppenheimer approx. for slow vs. fast d.o.f's.
  - ② Usually interested in energetically low-lying dynamics. At low  $T$ , universal behavior is more evident. Microscopic details not important  $\Rightarrow$  use simple model Hamiltonians.
  - ④ There are intrinsic symmetries - eg. time reversal, Galilean invariance, spin rotation, ...
    - symmetries imply conservation laws  $\rightarrow$  help to simplify and solve
    - but also tied to low-lying excitations: symmetry  $\rightarrow$  conservation law  $\rightarrow$  low-lying excitations
  - ③ Usually number of degrees of freedom (d.o.f.) is order  $10^{23}$   
 $\Rightarrow$  statistical treatments are useful (statistical errors negligible).

Oops: what about nuclei? Largest of order 300 protons + neutrons  $\ll 10^{23}$ !

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Footnote in AFS:

"The importance of this point is illustrated by the empirical observation that the most challenging systems in physical sciences are of medium (and not large) scale, eg. metallic clusters, medium-sized nuclei, or large atoms consist of  $O(10^2 - 10^3)$  fundamental constituents. Such problems are well beyond the reach of few-body quantum mechanics while not yet accessible to reliable statistical modeling. Often the only viable path to approaching systems of this type is massive use of phenomenology."

• But we want to calculate such systems systematically

\* • Attack from both ends

• few-body methods + extreme computing  $\Rightarrow$  much larger systems <sup>just briefly possible than implied above</sup>

• Use statistical framework  $\rightarrow$  path integral-based field theory <sup>most of our time</sup>

• effective actions are natural formalism for density

Function theory  $\rightarrow$  sub initio DFT. Partition function with great external sources: + Legendre transform

• Note historically looked to nuclear or neutron matter as simpler systems  $\rightarrow$  thermodynamic limit of nuclear interior (without Coulomb).

amenable to approximations, solving on computer

• How do AFS say to construct low-energy field theory?

(A) microscopic analysis

• Start from microscopic system and project on dof's believed most relevant for low-energy dynamics; identify small expansion parameter to justify.

(B) Symmetry considerations

• One infers effective low-energy theory based only on symmetries of the physical system

For us:

(A)  $\rightarrow$  renormalization group methods

(B)  $\rightarrow$  effective field theory

) can be combined!

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Handout: 1st 4 pages of review article by Furnstahl, Rupak, Schöber  
on "Effective Field Theory and Finite-Density Systems"

One goal: To be able to understand this article! (Not expected to understand yet!)

• We'll have something to say about every item in the table of contents (except "Ion physics from chiral EFT" → do as extra session)

• Here: Some big picture background + pictures for EFT and RG.

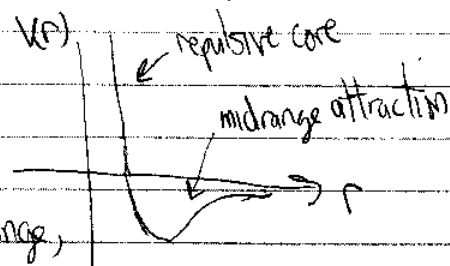
Consider "overview 1" handout with nucleon-nucleon and  ${}^3\text{He}$ - ${}^3\text{He}$  atomic potentials

- these are (effective) potentials between a neutron and a proton, or between two neutral  ${}^3\text{He}$  atoms as a function of separation. So potentials for composite objects, not fundamental interactions.
- note that NN potential is for relative orbital angular momentum  $L=0$  and total spin  $S=0 \Rightarrow \uparrow\downarrow S_0^{L=0}$  "singlet S-wave" state

$\Rightarrow$  potential is different for different  $L, S$  (and  $n, np, pp$ ), which complicates the nuclear problem!  $V(r)$

Note the similar qualitative features:

- very strong short-range repulsion
- attractive at intermediate range and long range, although the fall-off with  $r$  is much faster than Coulomb  $1/r$ .



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- Where do these potentials come from?
- One source is from a more fundamental underlying interaction
- In  $^3\text{He}$ , that interaction is quantum electrodynamics (QED), which reduces here primarily to the good old Coulomb interaction
- Each  $^3\text{He}$  is a few-body problem with Coulomb potential  $V_C(\vec{r}_a - \vec{r}_b) \propto -\frac{e^2}{|\vec{r}_a - \vec{r}_b|}$  between each of the two electrons and also a potential between the e's and the (assumed inert!) nucleus.
- Put two together and we can find the potential energy as a function of the separation of the nuclei
- First done variationally by Slater and Kirkwood in 1931  
[Exercise: look this up, in Physical Review 37 (1931) 682.  
One way: Google "Slater Kirkwood Physical Review"]
- Basic physics:
  - repulsion from Coulomb repulsion of overlapping electron clouds  $\Rightarrow$  very steep function of separation  $r$
  - attraction from induced electric dipoles: "mutual electric polarization" (2<sup>nd</sup>-order perturbation theory implies attraction if atoms are in their ground states:  $E^{(2)} = \sum_{j \neq 0} \frac{|\langle 0 | H | j \rangle|^2}{E_0 - E_j} < 0$ )

• Three questions: (for discussion)

- often Lennard-Jones  $-\frac{a}{r^6} + \frac{b}{r^{12}}$  potential used,  $1/r^6$  agrees with induced dipoles. What is theoretical motivation for  $1/r^6$ ?
  - None! Just for convenience. How can we can away with this?  $\Rightarrow$  later discussion of renormalization. (EFT exploits freedom to use convenient short range potential if we renormalize)
- How would you determine this potential experimentally?
  - Put two atoms at distance  $r$  and measure energy (or change in energy from far apart)? Doesn't work unless infinitely heavy atoms or far apart.  $\Rightarrow$  short-range part of the interaction is not an observable! (So can choose or transform many ways  $\rightarrow$  exploit with EFT and RG).
- Is the interaction of 3  $^3\text{He}$  atoms the sum of the pairwise potentials?  $H \stackrel{?}{=} H_1 + H_2 + H_3 + V_{12} + V_{23} + V_{13}$ ? No! More on this below...

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- For nuclear-nuclear case, we also know the underlying interaction for each  $\Rightarrow$  quantum chromodynamics (called QCD).
- Each nucleon is a composite system of quarks interacting via gluon exchange (cf. electrons interacting via photon exchange). But we don't have a simple analog to Coulomb.
- However, recently Aoki, Hatsuda, Ishii showed how to find the potential from lattice QCD [see back of "Overview 1"]
- Looks qualitatively reasonable (remember - not unique!)
- Long-range <sup>part</sup> is understood as originating from one-pion exchange (pion is a spin-zero meson with charge  $-1, +1$ , or  $0$  and rest mass of about  $140 \text{ MeV}/c^2$ ) as (essentially) a rigorous consequence of QCD (approximate goldstone boson of spontaneously and explicitly broken chiral symmetry - for experts only!)
- Effective shorter-range is more phenomenological
  - 2-pion exchange attraction (heavier, so shorter range)
  - vector (spin 1) meson  $\rho, \omega$  exchange  $\Rightarrow$  short-range repulsion (cf. spin-1 photon exchange between same charges)
- One of major tasks in the nuclear many-body problem has been to find this potential  $\Rightarrow$  we need the Hamiltonian to get started!
  - How do you know it is correct? Calculate experimental observables and compare to data.
    - One two-body bound state (deuteron)
    - lots of two-nucleon scattering data (phase shifts)
  - Several phenomenological potentials reproduce two-body data at energies up to inelastic processes (pion production) with  $\chi^2/\text{dof}$  of  $\approx 1$ . Not unique!
  - But fail to reproduce 3, 4, ... body data by 10% or more.  $\Rightarrow$  3 body forces
  - Chiral effective field theory to systematically build  $NN + NNN + NNNN + \dots$  interaction. [discussed as extra session]



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- What might we expect qualitatively from a many-body system with such a potential?
- Use your thermodynamics!
- Compare to ideal gas  $PV = nRT$  ( $n$  is # of moles)

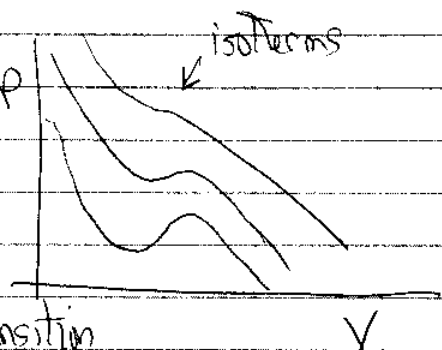
① Hard core repulsion means particles can't use entire volume (ie. "excluded volume") so  $[V \rightarrow V - nb]$  with  $b$  constant.

② Attraction means the pressure (on the container wall, for example) is reduced: net force on surface particle (next to wall) is proportional to number density and # of particles in surface region is also proportional to density  $\Rightarrow$  reduction goes like  $(\frac{n}{V})^2$ :

$$P = \frac{nRT}{V - nb} \rightarrow P = \frac{nRT}{V - nb} - \frac{an^2}{V^2}$$

$$\text{or } \left[ \left( P + \frac{an^2}{V^2} \right) (V - nb) = nRT \right]$$

$\Rightarrow$  Van der Waals equation of state



- Recall that there is a liquid-gas phase transition  $\Rightarrow$  there is one in the nuclear case.
- Probed in low-energy heavy-ion collisions.
- nucleus as liquid drop

- Liquid helium has very interesting physics at low  $T \Rightarrow$  it is superfluid
  - a consequence of the attractive interaction  $\Rightarrow$  pairing as in a superconductor (discuss later using effective actions)
  - liquid  $^3\text{He}$  very different from  $^4\text{He} \Rightarrow$  fermions vs. bosons is important!
- \* • nuclei also exhibit pairing!
  - How does this play out when only  $\sim 100$  particles?

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• Look at "overview" slide: "Degrees of Freedom: From QCD to Nuclei"

• on left is "periodic table" of atomic nuclei (called table of nuclides)

• How many are there? Answer: we don't know! Several thousands have been produced in lab, maybe as many as  $10^4$ .

• most are unstable to beta decay, fission,  $\alpha$ -decay

• many unmeasured/unseen important for stellar nucleosynthesis

⇒ new experimental facilities ("rare isotope beams") ⇒ FRIB, etc.

• Theoretical predictions will still be essential

• Note interactions below and methods above

• low-mom ⇒ low-momentum ⇒ here's where RG comes in

• degrees of freedom on right: like variables used

• at lower energies, more collective dof's to understand physics

• RG ⇒ focus on relevant dof's ⇒ don't want to use fine details (like quarks+gluons)

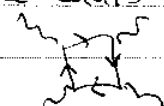
• on back, quote from Steven Weinberg

• essay "Why the RG is a Good Thing" is linked on web page.

Worth reading, although may be over your head at present.

• RG appears in many contexts, as given in bullets. May not seem like the same thing — common thread is relevant dof's.

• near-phase transitions, correlation length diverges, washing out short-distance details → eliminate these dof's

• in high energy  there is a "loop integral"

⇒ a sum over intermediate states. You don't want this sum to have large contributions from very different energies from the external states (eg. if 100 GeV photons, don't want 1 MeV electron energies to be important in calculation).

• RG lets you make this happen. Different types of implementation. Here we'll look at a visual one.

⇒ jump to overview-4 with "Computational Aside" and "Resolution Analogy"

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In "Computational Aside: Digital Potentials" we have a picture of a potential.

- Not like our previous pictures on overview-1!
- It is in momentum representation  $\langle k | \hat{V} | k' \rangle \xrightarrow{\text{discrete}} \langle k_i | \hat{V} | k_j \rangle \rightarrow \tilde{V}_{ij}$  matrix
- Calculations are just matrix multiplications



• "Resolution Analogy" shows two pictures of Abraham Lincoln.

- on the left is a photomosaic - lots of little high detail small pictures make up the large scale picture.

⇒ the "long distance" information - recognizing Lincoln - doesn't need this detail, which is distracting, takes lots of memory, and is even wrong!

• analogous to using the nuclear potential we looked at earlier!

- on the right is still recognizable, much less storage.

• achieved by "block spinning" → replace  by  average done by software in your browser.

• This is one way to do an RG! Eliminating short-distance dof's ⇒ "integrating out"

• On the back is another way: Fourier transform to momentum space.

- See how the two dimensional Fourier transforms encode the same information (not so recognizable!)

• In all pictures, can be represented as a matrix and the FT is accomplished by matrix multiplication

$$\langle k | V | k' \rangle = \int dx \int dx' \langle k | x \rangle \langle x | V | x' \rangle \langle x' | k' \rangle$$

$$\rightarrow \langle k_i | V | k_j \rangle = \sum_m \langle k_i | x_m \rangle \langle x_m | V | x_m \rangle \langle x_m | k_j \rangle \quad \text{by } m \text{ run from } 1 \text{ to } \# \text{ of } x \text{ points.}$$

$$\rightarrow \tilde{V}_{ij} = \sum_m F_{il}^\dagger V_{lm} F_{mj} \quad \text{or} \quad \underline{\tilde{V}} = \underline{F}^\dagger \underline{V} \underline{F} \quad \text{as matrices.}$$

- short distance detail ⇒ small wavelengths ⇒ large wave numbers.

• Just set to zero here, and relevant info in picture of woman is preserved. But not so easy in quantum mechanics ⇒ need additional transformations.

• One way to do this is called the Similarity Renormalization Group, or SRG.

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• This is shown in Overview-2 "For Atomic Nuclei, There's a Crowd"

• This is a slide that is supposed to be at a level suitable for congressional staff people. (!)

• It shows two things

a) practical consequence of using RG transformations

b) necessary consequence of using low-energy d.o.f's

Point b) is that there are three-body forces.

• Just like tides, can't add pairwise gravity forces because of tidal effects. [To think about: What does the effective two-body force/potential look like as a function of distance if tides are taken into account.]

• Same thing happens with atoms, but mostly negligible because  $\alpha \approx \frac{1}{137}$  is so small. (from 3rd order perturbation theory)

• On back, some additional info on three-body forces (like  $\pi$ -boson!) and one source for nuclear physics (the  $\Delta$  is an excited state of the nucleon, so this is like a polarization).

• Three-body <sup>potential</sup> is basically defined as what is left over when all pairwise two-body interactions are accounted for in a 3-body system.

Point a) is what the colored pictures show. This is a series of transformations of the  $\langle K|V|K' \rangle$  matrix to make it more diagonal.

This means  $\langle K_{high}|V|K_{low} \rangle \rightarrow 0$  so we can chop out  $K_{high}$ , just as in the 2D Fourier transform example.

• implemented as coupled first-order differential equations for the matrix elements.

• This is just the 2-body potential. Not shown is that the 3-body potential is also represented as a matrix and "evolves" to decouple high and low energy.

• The plot of the  ${}^4\text{He}$  (not a big system - 2 protons + 2 neutrons) ground state energy using matrix diagonalization. (More later).

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Clearly a smaller matrix will be faster.

• Matrix size is measured in " $N_{\max}$ " (explained later)

$N_{\max}$  "the matrix size (roughly)"

10 400

12 700

14 1500

16 2700

18 4800

• so big savings to converge by 8 or 10 rather than 16 or 18.

• But not so big matrices.

• However, grows very rapidly with nuclear size  $\Rightarrow$

$\Rightarrow$  see "overruns" plot of "matrix dimension"

vs. "Number of oscillator shells"

•  $10^8 - 10^9$  dimension is currently possible on large computer

• If  $N_{\max} = 1608$  is needed, too hopeless, but possible for  $^{16}O$  at least if  $N_{\max} = 608$  suffices.

• Many interesting details of solution method (Lanczos algorithm)

A nucleus,  
K orbitals:  
 $\sim K!$   
 $(K+1)A!$

• This wall of small numbers is why many-body texts turn to field theory methods (and quantization, path integrals, etc.)

• We will do so as well, but first a bit more on how we would solve these problems.

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• Return to  $\langle x|V|x' \rangle$  and ask: is potential unique?

• No. For example, it is local as given in the pictures.

One can construct non-local potentials that reproduce the same scattering and bound-state data.

Usual S-eqn (1-D)  
(eigenvalue eqn)

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + V(x) \psi(x) = E \psi(x)$$

• Kinetic energy term is nonlocal slightly:

discrete approximation:

$$\frac{d^2 \psi(x)}{dx^2} \rightarrow \frac{\psi(x_{i+1}) - 2\psi(x_i) + \psi(x_{i-1}))}{2\Delta x^2}$$

this is a  
sparse  
matrix so

$$\frac{1}{2\Delta x} \begin{pmatrix} 0 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix}$$

simple  
matrices

involves  $\psi(x)$  at nearby points in a simple way.

Do the same for  $V(x)$

(X)

$$V(x_i) \psi(x_i) \rightarrow \sum_j V(x_i, x_j) \psi(x_j) \rightarrow \left[ \int dx' V(x, x') \psi(x') \right] \text{ "nonlocal potential"}$$

matrix multiplication

• It is also energy independent (same potential no matter what relative energy of the particles).

• The potential is designed to fit scattering over a wide range of momenta. What if <sup>in</sup> ~~only~~ <sup>scattering</sup> low momenta?

• Low momentum  $\Rightarrow$  long wavelength

• of multipole expansion: at large wavelength, complicated charge or current distribution behaves like leading multipole (point charge or point dipole or ...)

$\Rightarrow$  replace complicated potential by simpler version that reproduces data in limited range.

$\Rightarrow$  basic idea of effective field theory and renormalization group methods we'll discuss is to do this systematically

Here, replace potential by delta function:  $V(\vec{x}, \vec{x}_0) = \lambda \delta(\vec{x}, \vec{x}_0)$  <sup>on right hand side, based on calculation</sup>  
Reproduces very low-energy scattering. Actually excellent for atoms in traps. <sup>two photon exchange</sup>

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So, given a potential, how do we solve a many-body problem?

The many-particle Hamiltonian ( $N$  particles) is

$$H = \sum_{i=1}^N T(x_i) + \frac{1}{2} \sum_{(i,j)=1}^N V(x_i, x_j)$$

$$= \sum_{i=1}^N T(x_i) + \sum_{i < j} V(x_i, x_j)$$

} avoid double counting

where  $T$  is the kinetic energy and  $V$  the potential energy.

(including any external one-body potential)

Here  $x_i \equiv \{\vec{x}_i, s_i, t_i, \dots\}$  denotes all coordinates of  $i^{\text{th}}$  particle.

• e.g.  $T(x_i) = -\frac{\hbar^2 \nabla_i^2}{2m}$  usually

• Then time-dependent S-eqn is

$$i\hbar \frac{\partial}{\partial t} \Psi(x_1, \dots, x_N; t) = H \Psi(x_1, \dots, x_N; t)$$

[Note: If we know the operators]

• If we find  $\Psi$  (or the energy eigenstates), we can calculate all we want!

• How might we solve this? Enumerate  $N=1$  methods!

which methods generalize to many-body?

• solve differential equation in coordinate space (integro-diff eq in general)  
 $\Rightarrow$  very hard when multidimensional

• solve integral equation in momentum space

• write  $H = H_0 + H_1$  with  $H_0$  solvable and do perturbation theory in  $H_1$  (one choice is  $H_0 = T$ ,  $H_1 = V$ )

• diagonalize  $H$  in a complete basis (or an over-complete basis — see SVM!)

• use the variational principle: minimize  $\langle \Psi_{\text{trial}} | H | \Psi_{\text{trial}} \rangle$  with respect to parameters in trial wave function  $|\Psi_{\text{trial}}\rangle$

diagonalizing in basis is special case of variational — parameters are coefficients of basis states

• project out the ground state starting from a wave function  $|\Psi_0\rangle$  with non-zero overlap by applying  $e^{-H\tau} |\Psi_0\rangle$

• e.g. in one-d with one particle,

$$\Psi_0(x) = a_0 \psi_0(x) + a_1 \psi_1(x) + \dots \quad \text{where } H \psi_i(x) = E_i \psi_i(x) \text{ are exact eigenstates}$$

$$\text{then } e^{-H\tau} \Psi_0(x) = a_0 e^{-E_0 \tau} \psi_0(x) + a_1 e^{-E_1 \tau} \psi_1(x) + \dots \xrightarrow{\tau \rightarrow \infty} a_0 e^{-E_0 \tau} \psi_0(x)$$

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• This might remind you of two things!

- i) a Boltzmann factor  $e^{\beta H} \Rightarrow \beta \leftrightarrow \frac{1}{T}$
- ii) formal solution to time evolution

$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = \hat{H} \Psi(x,t) \Rightarrow \Psi(x,t) = e^{-i\hat{H}t/\hbar} \Psi(x,0)$$

$\Rightarrow$  evolution in imaginary time!

- We'll see both connections soon with path integrals.  
(How can we compute  $\text{Tr } e^{\beta H}$ ?)

• But first we'll consider a matrix diagonalization method called the "stochastic Variational Method" or SVM

- See handout of paper by Blume et al. For recent application to look at universal behavior (eg. in cold atoms)
- Build many-body basis wave functions from gaussian functions (eg. in coordinate space)

$\Rightarrow$  matrix elements can be calculated (usually) analytically

- Variational parameters are widths of gaussians:  $A$  or  $A_{ij}$  below

- $N=1$  particle  $\Psi(x) \propto e^{-Ax^2}$ ,  $A$  a constant

- $N$  particles  $\Psi(x_1, x_2, \dots, x_N) \propto e^{-\sum_{i,j=1}^N x_i A_{ij} x_j} \rightarrow e^{-\underline{x}^T \underline{A} \underline{x}} = \Psi(\underline{A})$

- Stochastic  $\Rightarrow$  choose  $A_{ij}$ 's at random!!

- keep those that lower the energy (since a variational energy is an upper bound)

- Non-orthogonal basis of size  $K$

$$\Psi(\underline{x}) = \sum_{i=1}^K c_i \Psi(\underline{A}_i)$$

$\Rightarrow$  energy from generalized eigenvalue problem

$$\sum_{j=1}^K (H_{ij} - E B_{ij}) c_j = 0 \quad (i=1, \dots, K)$$

where

$$H_{ij} = \langle \Psi(\underline{A}_i) | H | \Psi(\underline{A}_j) \rangle, \quad B_{ij} = \langle \Psi(\underline{A}_i) | \Psi(\underline{A}_j) \rangle.$$