Second Quantization
and
Jordan-Wigner Representations

Erik Koch
Jülich Supercomputer Centre

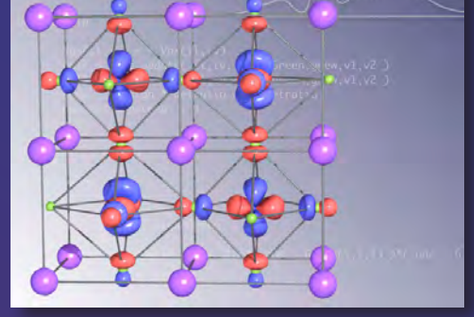
$$\Phi_{\alpha_1\alpha_2\ldots\alpha_N}(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{N!}} \left\langle 0 \middle| \hat{\psi}(x_1)\hat{\psi}(x_2)\ldots\hat{\psi}(x_N) \;\; c^\dagger_{\alpha_N}\ldots c^\dagger_{\alpha_2} c^\dagger_{\alpha_1} \middle| 0 \right\rangle$$

$$c_\alpha|0\rangle = 0 \qquad \left\{c_\alpha, c_\beta\right\} = 0 = \left\{c^\dagger_\alpha, c^\dagger_\beta\right\}$$

$$\langle 0|0\rangle = 1 \qquad \left\{c_\alpha, c^\dagger_\beta\right\} = \langle\alpha|\beta\rangle$$

$$c_i^\dagger \to \sigma_i^+ \otimes (-\sigma_{i-1}^z) \otimes \cdots \otimes (-\sigma_1^z)$$
$$c_i \to \sigma_i^- \otimes (-\sigma_{i-1}^z) \otimes \cdots \otimes (-\sigma_1^z)$$

Autumn School on Correlated Electrons



Simulating Correlations with Computers

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Simulating Physics with Computers

Richard P. Feynman

Department of Physics, California Institute of Technology, Pasadena, California 91107

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The Theory of Everything

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R. B. Laughlin* and David Pines†‡§

*Department of Physics, Stanford University, Stanford, CA 94305; †Institute for Complex Adaptive Matter, University of California Office of the President, Oakland, CA 94607; ‡Science and Technology Center for Superconductivity, University of Illinois, Urbana, IL 61801; and §Los Alamos Neutron Science Center Division, Los Alamos National Laboratory, Los Alamos, NM 87545

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We discuss recent developments in our understanding of matter, broadly construed, and their implications for contemporary research in fundamental physics.

The Theory of Everything is a term for the ultimate theory of the universe—a set of equations capable of describing all phenomena that have been observed, or that will ever be observed (1). It is the modern incarnation of the reductionist ideal of the ancient Greeks, an approach to the natural world that has been fabulously successful in bettering the lot of mankind and continues in many people's minds to be the central paradigm of physics. A special case of this idea, and also a beautiful instance of it, is the equation of conventional nonrelativistic quantum mechanics, which describes the everyday world of human beings—air, water, rocks, fire, people, and so forth. The details of this equation are less important than the fact that it can be written down simply and is completely specified by a handful of known quantities: the charge and mass of the electron, the charges and masses of the atomic nuclei, and Planck's constant. For experts we write

$$i\hbar\,\frac{\partial}{\partial t}\,|\Psi> \;=\; \mathcal{H}|\Psi> \qquad [1]$$

where

$$\mathcal{H} = -\sum_{j}^{N_e}\frac{\hbar^2}{2m}\nabla_j^2 - \sum_{\alpha}^{N_i}\frac{\hbar^2}{2M_\alpha}\nabla_\alpha^2 - \sum_{j}^{N_e}\sum_{\alpha}^{N_i}\frac{Z_\alpha e^2}{|\vec{r}_j-\vec{R}_\alpha|} + \sum_{j\ll k}^{N_e}\frac{e^2}{|\vec{r}_j-\vec{r}_k|} + \sum_{\alpha\ll\beta}^{N_j}\frac{Z_\alpha Z_\beta e^2}{|\vec{R}_\alpha-\vec{r}_\beta|}. \qquad [2]$$

we have learned why atoms have the size they do, why chemical bonds have the length and strength they do, why solid matter has the elastic properties it does, why some things are transparent while others reflect or absorb light (6). With a little more experimental input for guidance it is even possible to predict atomic conformations of small molecules, simple chemical reaction rates, structural phase transitions, ferromagnetism, and sometimes even superconducting transition temperatures (7). But the schemes for approximating are not first-principles deductions but are rather art keyed to experiment, and thus tend to be the least reliable precisely when reliability is most needed, i.e., when experimental information is scarce, the physical behavior has no precedent, and the key questions have not yet been identified. There are many notorious failures of alleged *ab initio* computation methods, including the phase diagram of liquid ^{3}He and the entire phenomenonology of high-temperature superconductors (8–10). Predicting protein functionality or the behavior of the human brain from these equations is patently absurd. So the triumph of the reductionism of the Greeks is a pyrrhic victory: We have succeeded in reducing all of ordinary physical behavior to a simple, correct Theory of Everything only to discover that it has revealed exactly nothing about many things of great importance.

In light of this fact it strikes a thinking person as odd that the parameters e, $\hbar$, and m appearing in these equations may be measured accurately in laboratory experiments involving large numbers of particles. The electron charge, for example, may be accurately measured by passing current through an electrochemical cell, plating out metal atoms, and measuring the mass deposited, the separation of the atoms in the crystal being known from x-ray diffraction (11). Simple electrical measurements performed on superconducting rings determine to high accuracy the quantity the quantum of magnetic flux $hc/2e$ (11). A version

Theory of Almost Everything

given Hamiltonian

$$H = -\frac{1}{2}\sum_{j=1}^{N_e}\nabla_j^2 + \sum_{j<k}^{N_e}\frac{1}{|r_j - r_k|} - \sum_{j=1}^{N_e}\sum_{\alpha=1}^{N_i}\frac{Z_\alpha}{|r_j - R_\alpha|} + \sum_{\alpha<\beta}^{N_i}\frac{Z_\alpha Z_\beta}{|R_\alpha - R_\beta|}$$

solve eigenvalue problem

$$H\Psi(x_1, \ldots, x_N) = E\,\Psi(x_1, \ldots, x_N)$$

3*N*-dimensional pde

electrons indistinguishable — how possible?

no observable $M(x_1,\ldots,x_N)$ can distinguish them
i.e. M symmetric under exchange of coordinates

eigenfunction needs to be antisymmetrized — still eigenfunction?

$$\mathcal{A}\,\Psi(x_1, \ldots, x_N) := \frac{1}{N!}\sum_{P}(-1)^P \Psi\left(x_{p(1)}, \ldots, x_{p(N)}\right)$$

N! terms

antisymmetrization

$$\mathcal{A}\,\psi(x_1,\ldots,x_N) := \frac{1}{N!}\sum_P (-1)^P \psi\left(x_{p(1)},\ldots,x_{p(N)}\right)$$

$N!$ terms — hard problem in general
easy $O(N^3)$ for product wavefunctions

$$\sqrt{N!}\,\mathcal{A}\,\varphi_{\alpha_1}(x_1)\cdots\varphi_{\alpha_N}(x_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \varphi_{\alpha_1}(x_1) & \varphi_{\alpha_2}(x_1) & \cdots & \varphi_{\alpha_N}(x_1) \\ \varphi_{\alpha_1}(x_2) & \varphi_{\alpha_2}(x_2) & \cdots & \varphi_{\alpha_N}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_{\alpha_1}(x_N) & \varphi_{\alpha_2}(x_N) & \cdots & \varphi_{\alpha_N}(x_N) \end{vmatrix}$$

Slater determinants $\Phi_{\alpha_1,\ldots,\alpha_N}(x_1,\ldots,x_N)$

basis of Slater determinants

complete set of single-electron orbitals

$$\sum_n \overline{\varphi_n(x')}\,\varphi_n(x) = \delta(x'-x)$$

expand N-electron function in 1st variable

$$a(x_1,\ldots,x_N) = \sum_{n_1}\int dx_1'\ \underbrace{a(x_1',\ldots,x_N)\,\overline{\varphi_{n_1}(x_1')}}_{=:a_{n_1}(x_2,\ldots,x_N)}\ \varphi_{n_1}(x_1)$$

and repeat to obtain expansion in product states

antisymmetric: states with $n_i{=}n_j$ vanish, $n_i{\leftrightarrow}n_j$ only differ by sign

basis of Slater determinants

$$\left\{\Phi_{n_1,\ldots,n_N}(x_1,\ldots,x_N)\,\middle|\ n_1<n_2<\cdots<n_N\right\}$$

second quantization: motivation

get rid of coordinates and their permutations: Dirac states

Slater determinant $$\Phi_{\alpha\beta}(x_1, x_2) = \frac{1}{\sqrt{2}} \left(\varphi_\alpha(x_1)\varphi_\beta(x_2) - \varphi_\beta(x_1)\varphi_\alpha(x_2)\right)$$

corresponding Dirac state $$|\alpha, \beta\rangle = \frac{1}{\sqrt{2}} \left(|\alpha\rangle|\beta\rangle - |\beta\rangle|\alpha\rangle\right)$$

use operators $$|\alpha, \beta\rangle = c_\beta^\dagger c_\alpha^\dagger |0\rangle$$

position of operators encodes signs

$$c_\beta^\dagger c_\alpha^\dagger |0\rangle = |\alpha, \beta\rangle = -|\beta, \alpha\rangle = -c_\alpha^\dagger c_\beta^\dagger |0\rangle$$

product of operators changes sign under commutation: anti-commutation

anti-commutator $$\{A, B\} := A\,B + B\,A$$

second quantization: motivation

specify *N*-electron states using operators

N=0: $|0\rangle$ (vacuum state)

normalization: $\langle 0|0\rangle = 1$

N=1: $|\alpha\rangle = c_\alpha^\dagger|0\rangle$ (creation operator adds one electron)

normalization: $\langle\alpha|\alpha\rangle = \langle 0|c_\alpha c_\alpha^\dagger|0\rangle$

overlap: $\langle\alpha|\beta\rangle = \langle 0|c_\alpha c_\beta^\dagger|0\rangle$

adjoint of creation operator must remove one electron: annihilation operator

$$c_\alpha|0\rangle = 0 \text{ and } c_\alpha c_\beta^\dagger = \pm c_\beta^\dagger c_\alpha + \langle\alpha|\beta\rangle$$

N=2: $|\alpha,\beta\rangle = c_\beta^\dagger c_\alpha^\dagger|0\rangle$

antisymmetry: $c_\alpha^\dagger c_\beta^\dagger = -c_\beta^\dagger c_\alpha^\dagger$

second quantization: formalism

vacuum state $|0\rangle$

and

set of operators c_α related to single-electron states $\varphi_\alpha(x)$

defined by:

$$c_\alpha|0\rangle = 0 \qquad \left\{c_\alpha, c_\beta\right\} = 0 = \left\{c_\alpha^\dagger, c_\beta^\dagger\right\}$$

$$\langle 0|0\rangle = 1 \qquad \left\{c_\alpha, c_\beta^\dagger\right\} = \langle\alpha|\beta\rangle$$

creators/annihilators operate in Fock space
transform like orbitals

second quantization: field operators

how to express coordinates?
creation/annihilation operators in real-space basis

$\hat{\psi}^\dagger(x)$ with $x = (r, \sigma)$ creates electron of spin σ at position r

then $c_\alpha^\dagger = \int dx\, \varphi_\alpha(x) \hat{\psi}^\dagger(x)$

put electron at x with amplitude $\varphi_a(x)$

$\{\varphi_{\alpha_n}(x)\}$ complete set: $\hat{\psi}^\dagger(x) = \sum_n \overline{\varphi_{\alpha_n}(x)}\, c_{\alpha_n}^\dagger$

they fulfill the standard anti-commutation relations

$$\{\hat{\psi}(x), \hat{\psi}(x')\} = 0 = \{\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(x')\}$$
$$\{\hat{\psi}(x), \hat{\psi}^\dagger(x')\} = \delta(x - x')$$

second quantization: Slater determinants

$$\Phi_{\alpha_1\alpha_2\ldots\alpha_N}(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{N!}} \left\langle 0 \left| \hat{\psi}(x_1)\hat{\psi}(x_2)\ldots\hat{\psi}(x_N)\, c^\dagger_{\alpha_N}\ldots c^\dagger_{\alpha_2} c^\dagger_{\alpha_1} \right| 0 \right\rangle$$

proof by induction

N=1: $\left\langle 0 \left| \hat{\psi}(x_1)\, c^\dagger_{\alpha_1} \right| 0 \right\rangle = \left\langle 0 \left| \varphi_{\alpha_1}(x_1) - c^\dagger_{\alpha_1}\hat{\psi}(x_1) \right| 0 \right\rangle = \varphi_{\alpha_1}(x_1)$

using $\{\hat{\psi}(x), c^\dagger_\alpha\} = \int dx'\, \varphi_\alpha(x') \left\{\hat{\psi}(x), \hat{\psi}^\dagger(x')\right\} = \varphi_\alpha(x)$

N=2: $\left\langle 0 \left| \hat{\psi}(x_1)\hat{\psi}(x_2)\, c^\dagger_{\alpha_2} c^\dagger_{\alpha_1} \right| 0 \right\rangle$

$$= \left\langle 0 \left| \hat{\psi}(x_1) \left(\varphi_{\alpha_2}(x_2) - c^\dagger_{\alpha_2}\hat{\psi}(x_2)\right) c^\dagger_{\alpha_1} \right| 0 \right\rangle$$

$$= \left\langle 0 \left| \hat{\psi}(x_1) c^\dagger_{\alpha_1} \right| 0 \right\rangle \varphi_{\alpha_2}(x_2) - \left\langle 0 \left| \hat{\psi}(x_1) c^\dagger_{\alpha_2}\hat{\psi}(x_2) c^\dagger_{\alpha_1} \right| 0 \right\rangle$$

$$= \varphi_{\alpha_1}(x_1)\varphi_{\alpha_2}(x_2) - \varphi_{\alpha_2}(x_1)\varphi_{\alpha_1}(x_2)$$

second quantization: Slater determinants

general N: commute $\Psi(x_N)$ to the right

$$\left\langle 0 \left| \hat{\psi}(x_1) \ldots \hat{\psi}(x_{N-1}) \hat{\psi}(x_N)\, c^\dagger_{\alpha_N} c^\dagger_{\alpha_{N-1}} \ldots c^\dagger_{\alpha_1} \right| 0 \right\rangle \;=$$

$$\begin{aligned}
&+ \quad \left\langle 0 \left| \hat{\psi}(x_1) \ldots \hat{\psi}(x_{N-1})\, c^\dagger_{\alpha_{N-1}} \ldots c^\dagger_{\alpha_1} \right| 0 \right\rangle \; \varphi_{\alpha_N}(x_N) \\
&- \quad \left\langle 0 \left| \hat{\psi}(x_1) \ldots \hat{\psi}(x_{N-1}) \prod_{n \neq N-1} c^\dagger_{\alpha_n} \right| 0 \right\rangle \; \varphi_{\alpha_{N-1}}(x_N) \\
&\;\;\vdots \\
&(-1)^{N-1} \left\langle 0 \left| \hat{\psi}(x_1) \ldots \hat{\psi}(x_{N-1})\, c^\dagger_{\alpha_N} \quad \ldots \quad c^\dagger_{\alpha_2} \right| 0 \right\rangle \; \varphi_{\alpha_1}(x_N)
\end{aligned}$$

Laplace expansion in terms of $N-1$ dim determinants wrt last line of

$$= \begin{vmatrix}
\varphi_{\alpha_1}(x_1) & \varphi_{\alpha_2}(x_1) & \cdots & \varphi_{\alpha_N}(x_1) \\
\varphi_{\alpha_1}(x_2) & \varphi_{\alpha_2}(x_2) & \cdots & \varphi_{\alpha_N}(x_2) \\
\vdots & \vdots & \ddots & \vdots \\
\varphi_{\alpha_1}(x_N) & \varphi_{\alpha_2}(x_N) & \cdots & \varphi_{\alpha_N}(x_N)
\end{vmatrix}$$

second quantization: Dirac notation

separate coordinates from orbitals

$$\Phi_{\alpha_1\alpha_2\ldots\alpha_N}(x_1, x_2, \ldots, x_N) = \frac{1}{\sqrt{N!}} \left\langle 0 \left| \hat{\psi}(x_1)\hat{\psi}(x_2)\cdots\hat{\psi}(x_N) \right. c^\dagger_{\alpha_N} \cdots c^\dagger_{\alpha_2} c^\dagger_{\alpha_1} \left| 0 \right\rangle \right.$$

analogous to Dirac notation

$$\varphi_\alpha(x) = \langle x|\alpha\rangle$$

product states $\prod_{n=1}^{N} c^\dagger_{\alpha_n}|0\rangle$ are many-body generalization of Dirac states

evaluate matrix elements …

second quantization: expectation values

expectation value of operator wrt *N*-electron Slater determinants

$$\int dx_1 \cdots dx_N \, \overline{\Phi_{\beta_1 \cdots \beta_N}(x_1, \cdots, x_N)} \, M(x_1, \cdots, x_N) \, \Phi_{\alpha_1 \cdots \alpha_N}(x_1, \cdots, x_N)$$

$$= \int d\boldsymbol{x} \, \frac{1}{\sqrt{N!}} \langle 0 | \prod c_{\beta_i} \prod \hat{\psi}^\dagger(x_n) | 0 \rangle \, M(\boldsymbol{x}) \, \frac{1}{\sqrt{N!}} \langle 0 | \prod \hat{\psi}(x_n) \prod c^\dagger_{\alpha_j} | 0 \rangle$$

$$= \langle 0 | \prod c_{\beta_i} \underbrace{\frac{1}{N!} \int d\boldsymbol{x} \, \prod \hat{\psi}^\dagger(x_n) \, M(\boldsymbol{x}) \, \prod \hat{\psi}(x_n)}_{=: \hat{M}} \prod c^\dagger_{\alpha_j} | 0 \rangle$$

$|0\rangle\langle 0| = \mathbb{1}$ on 0-electron space

$$\hat{M} = \frac{1}{N!} \int dx_1 \cdots dx_N \, \hat{\psi}^\dagger(x_N) \cdots \hat{\psi}^\dagger(x_1) \, M(x_1, \cdots, x_N) \, \hat{\psi}(x_1) \cdots \hat{\psi}(x_N)$$

only valid for *N*-electron states!

second quantization: zero-body operator

zero-body operator $M(x_1,\ldots x_N) = 1$ independent of particle coordinates

second quantized form for operating on N-electron states:

$$\hat{M}_0 = \frac{1}{N!}\int dx_1 dx_2 \cdots x_N\, \hat{\psi}^\dagger(x_N)\cdots\hat{\psi}^\dagger(x_2)\hat{\psi}^\dagger(x_1)\,\hat{\psi}(x_1)\hat{\psi}(x_2)\cdots\hat{\psi}(x_N)$$

$$= \frac{1}{N!}\int \quad dx_2 \cdots x_N\, \hat{\psi}^\dagger(x_N)\cdots\hat{\psi}^\dagger(x_2) \qquad \hat{N} \qquad \hat{\psi}(x_2)\cdots\hat{\psi}(x_N)$$

$$= \frac{1}{N!}\int \quad dx_2 \cdots x_N\, \hat{\psi}^\dagger(x_N)\cdots\hat{\psi}^\dagger(x_2) \qquad 1 \qquad \hat{\psi}(x_2)\cdots\hat{\psi}(x_N)$$

$$\vdots$$

$$= \frac{1}{N!}\, 1\cdot 2\, \cdots\, N = 1$$

only(!) when operating on N-electron state

using $\hat{N} := \int dx\, \hat{\psi}^\dagger(x)\hat{\psi}(x)$ with $\left[\hat{N},\, c_n^\dagger\right] = c_n^\dagger$

result independent of N

overlap of Slater determinants

$$\int dx\, \overline{\Phi_{\alpha_n}(x)}\,\Phi_{\beta_m}(x) = \langle 0|c_{\alpha_1}\cdots c_{\alpha_N}\; c^\dagger_{\beta_N}\cdots c^\dagger_{\beta_1}|0\rangle$$

second quantization: one-body operators

one-body operator $M(x_1, \ldots, x_N) = \sum_j M_1(x_j)$

$$\hat{M}_1 = \frac{1}{N!} \int dx_1 \cdots dx_N \, \hat{\psi}^\dagger(x_N) \cdots \hat{\psi}^\dagger(x_1) \sum_j M_1(x_j) \; \hat{\psi}(x_1) \cdots \hat{\psi}(x_N)$$

$$= \frac{1}{N!} \sum_j \int dx_j \, \hat{\psi}^\dagger(x_j) \, M_1(x_j) \, (N-1)! \; \hat{\psi}(x_j)$$

$$= \frac{1}{N} \sum_j \int dx_j \, \hat{\psi}^\dagger(x_j) \, M_1(x_j) \, \hat{\psi}(x_j)$$

$$= \int dx \quad \hat{\psi}^\dagger(x) \;\; M_1(x) \;\; \hat{\psi}(x)$$

result independent of *N*

expand in complete orthonormal set of orbitals

$$\hat{M}_1 = \sum_{n,m} \int dx \, \overline{\varphi_{\alpha_n}(x)} \, M(x) \, \varphi_{\alpha_m}(x) \; c^\dagger_{\alpha_n} c_{\alpha_m} = \sum_{n,m} \langle \alpha_n | M_1 | \alpha_m \rangle \; c^\dagger_{\alpha_n} c_{\alpha_m}$$

transforms as 1-body operator

second quantization: two-body operators

two-body operator $\quad M(x_1,\ldots,x_N)=\sum_{i<j} M_2(x_i,x_j)$

$$\hat{M}_2=\frac{1}{N!}\int dx_1\cdots dx_N\,\hat{\psi}^\dagger(x_N)\cdots\hat{\psi}^\dagger(x_1)\sum_{i<j}M_2(x_i,x_j)\;\hat{\psi}(x_1)\cdots\hat{\psi}(x_N)$$

$$=\frac{1}{N!}\sum_{i<j}\int dx_i dx_j\,\hat{\psi}^\dagger(x_j)\hat{\psi}^\dagger(x_i)\,M_2(x_i,x_j)\,(N-2)!\;\hat{\psi}(x_i)\hat{\psi}(x_j)$$

$$=\frac{1}{N(N-1)}\sum_{i<j}\int dx_i dx_j\,\hat{\psi}^\dagger(x_j)\hat{\psi}^\dagger(x_i)\,M_2(x_i,x_j)\,\hat{\psi}(x_i)\hat{\psi}(x_j)$$

$$=\frac{1}{2}\int dx\;dx'\;\hat{\psi}^\dagger(x')\;\hat{\psi}^\dagger(x)\;\;M_2(x,x')\;\;\hat{\psi}(x)\;\hat{\psi}(x')$$

result independent of N

expand in complete orthonormal set of orbitals

$$\hat{M}_2=\frac{1}{2}\sum_{n,n',m,m'}\int dxdx'\,\overline{\varphi_{\alpha_{n'}}(x')\varphi_{\alpha_n}(x)}\,M_2(x,x')\,\varphi_{\alpha_m}(x)\varphi_{\alpha_{m'}}(x')\;c^\dagger_{\alpha_{n'}}c^\dagger_{\alpha_n}c_{\alpha_m}c_{\alpha_{m'}}$$

$$=\frac{1}{2}\sum_{n,n',m,m'}\qquad\qquad\langle\alpha_n\alpha_{n'}|M_2|\alpha_m\alpha_{m'}\rangle\qquad\qquad c^\dagger_{\alpha_{n'}}c^\dagger_{\alpha_n}c_{\alpha_m}c_{\alpha_{m'}}$$

2-body matrix

$$\hat{M}_2 = \frac{1}{2} \sum_{n,n',m,m'} \underbrace{\langle \alpha_n \alpha_{n'} | M_2 | \alpha_m \alpha_{m'} \rangle}_{=: M_{nn',mm'}} c^\dagger_{\alpha_{n'}} c^\dagger_{\alpha_n} c_{\alpha_m} c_{\alpha_{m'}}$$

4-index tensor

no contribution for
n=*n*' or *m*=*m*'
sign-change for
n↔*n*' or *m*↔*m*'

no self-interaction

exchange terms

collect terms with same operator content

$$\hat{M}_2 = \sum_{n<n',m<m'} \left(\underbrace{M_{nn',mm'} - M_{nn',m'm}}_{=: \breve{M}_{nn',mm'}} \right) c^\dagger_{\alpha_{n'}} c^\dagger_{\alpha_n} c_{\alpha_m} c_{\alpha_{m'}}$$

two-body matrix
of dim $N_{orb}(N_{orb}-1)/2$

together with N_{orb}^2 hopping terms
completely specifies Hamiltonian

Exact Diagonalization

variational principle and Schrödinger equation

energy expectation value $E[\psi] = \dfrac{\langle\psi|H|\psi\rangle}{\langle\Psi|\Psi\rangle}$

variation

$$E[\Psi+\delta\Psi] = E[\Psi]+\frac{\langle\delta\Psi|H|\Psi\rangle + \langle\Psi|H|\delta\Psi\rangle}{\langle\Psi|\Psi\rangle} - \langle\Psi|H|\Psi\rangle \frac{\langle\delta\Psi|\Psi\rangle + \langle\Psi|\delta\Psi\rangle}{\langle\Psi|\Psi\rangle^2} + \mathcal{O}^2$$

variational equation: $0 = \dfrac{\delta E[\Psi]}{\delta\Psi} = \dfrac{H|\Psi\rangle - \overbrace{\langle\Psi|H|\Psi\rangle}^{=E[\Psi]}\ |\Psi\rangle}{\langle\Psi|\Psi\rangle} + \text{H.c.}$

equivalent to eigenvalue equation

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle$$

variational principle

expand $|\Psi\rangle \neq 0$ in eigenfunctions

$$E[\Psi] = \frac{\sum \langle\Psi|\Psi_m\rangle\langle\Psi_m|H|\Psi_n\rangle\langle\Psi_n|\Psi\rangle}{\sum \langle\Psi|\Psi_m\rangle\langle\Psi_m|\Psi_n\rangle\langle\Psi_n|\Psi\rangle} = \frac{\sum E_n \left|\langle\Psi_n|\Psi\rangle\right|^2}{\sum \left|\langle\Psi_n|\Psi\rangle\right|^2} \geq \frac{\sum E_0 \left|\langle\Psi_n|\Psi\rangle\right|^2}{\sum \left|\langle\Psi_n|\Psi\rangle\right|^2} = E_0$$

assume eigenvalues sorted $E_0 \leq E_1 \leq \ldots$

$$E[\Psi_{\perp_n}] \geq E_n \quad \text{if } \langle\Psi_i|\Psi_{\perp_n}\rangle = 0 \text{ for } i = 0, \ldots, n{-}1.$$

variational principle for excited states

in practice only useful when orthogonality to (unknown) states ensured, e.g., by symmetry

expand in Slater basis

rewrite $H|\Psi_n\rangle = E_n|\Psi_n\rangle$

choose (orthonormal) orbital basis $\{ \varphi_k \mid k \}$ and corresponding basis of Slater determinants $\{ \phi_{k1,\ldots,kN} \mid k_1 < \ldots < k_N \}$

$$|\Psi\rangle = \sum_{k_1<\cdots<k_N} a_{k_1,\ldots,k_N} |\Phi_{k_1,\ldots,k_N}\rangle = \sum_i a_i |\Phi_i\rangle = |\mathbf{\Phi}\rangle \boldsymbol{a}$$

expand Schrödinger equation in Slater basis

$$E \langle\Phi_i|\Psi\rangle = \langle\Phi_i|H|\Psi\rangle = \sum_j \langle\Phi_i|H|\Phi_j\rangle\langle\Phi_j|\Psi\rangle$$

matrix eigenvalue problem

$$\boldsymbol{H}\boldsymbol{a} = \langle\mathbf{\Phi}|\hat{H}|\mathbf{\Phi}\rangle\boldsymbol{a} = \begin{pmatrix} \langle\Phi_1|\hat{H}|\Phi_1\rangle & \langle\Phi_1|\hat{H}|\Phi_2\rangle & \cdots \\ \langle\Phi_2|\hat{H}|\Phi_1\rangle & \langle\Phi_2|\hat{H}|\Phi_2\rangle & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} = E \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix} = E\boldsymbol{a}$$

variational principle

restrict to finite Slater basis $|\tilde{\mathbf{\Phi}}\rangle := \left(|\Phi_1\rangle, \ldots, |\Phi_{\tilde{L}}\rangle\right)$

$$\langle\tilde{\mathbf{\Phi}}|\hat{H}|\tilde{\mathbf{\Phi}}\rangle\tilde{\boldsymbol{a}}_n = \tilde{\boldsymbol{H}}\tilde{\boldsymbol{a}}_n = \tilde{E}_n\tilde{\boldsymbol{a}}_n \quad \rightsquigarrow \quad |\tilde{\Psi}_n\rangle := |\tilde{\mathbf{\Phi}}\rangle\,\tilde{\boldsymbol{a}}_n$$

solve with LAPACK

variational principle: $E_n \leq \tilde{E}_n$ for $n \in \{0, \ldots, \tilde{L}-1\}$

construct $|\tilde{\Psi}\rangle = \sum_{i=0}^{n} c_i\,|\tilde{\Psi}_i\rangle \neq 0$ with $\langle\Psi_i|\tilde{\Psi}\rangle = 0$ for $i=0, \ldots, n-1$

$$\rightsquigarrow\ \tilde{E}_n\ \geq\ E[\tilde{\Psi}]\ \geq\ E_n$$

art: systematically increase basis to achieve convergence

nesting of eigenvalues

consider problem with basis size L as exact problem

variational principle for $-H$: $-E_{L-i} \leq -\tilde{E}_{\tilde{L}-i}$ for $i \in \{1, \ldots, \tilde{L}\}$

$$E_n \leq \tilde{E}_n \leq E_{n+(L-\tilde{L})} \quad \text{for } n \in \{0, \ldots, \tilde{L}-1\}$$

representation of basis

$$|n_{K-1}, \ldots, n_0\rangle := \prod_{k=0}^{K-1} \left(c_k^\dagger\right)^{n_k} |0\rangle$$

occupation number representation

i	(n_3, n_2, n_1, n_0)	state	I
0	0000		
1	0001		
2	0010		
3	0011	$c_1^\dagger c_0^\dagger \|0\rangle = \|\Phi_1\rangle$	1
4	0100		
5	0101	$c_2^\dagger c_0^\dagger \|0\rangle = \|\Phi_2\rangle$	2
6	0110	$c_2^\dagger c_1^\dagger \|0\rangle = \|\Phi_3\rangle$	3
7	0111		
8	1000		
9	1001	$c_3^\dagger c_0^\dagger \|0\rangle = \|\Phi_4\rangle$	4
10	1010	$c_3^\dagger c_1^\dagger \|0\rangle = \|\Phi_5\rangle$	5
11	1011		
12	1100	$c_3^\dagger c_2^\dagger \|0\rangle = \|\Phi_6\rangle$	6
13	1101		
14	1110		
15	1111		

bit-representation of basis states

```
>>> for i in range(2**4):
...   if bin(i).count('1')==2:
...     print(format(i, "04b"))
...
0011
0101
0110
1001
1010
1100
```

matrix elements: Fermi signs

$$\langle \Phi_I | \hat{H} | \Phi_{I'} \rangle = \sum_{n,m} T_{nm} \langle 0 | c_{I_1} \cdots c_{I_N} \, c_n^\dagger c_m \, c_{I'_N}^\dagger \cdots c_{I'_1}^\dagger | 0 \rangle$$

$$+ \sum_{\substack{n'>n \\ m'>m}} \breve{U}_{nn',mm'} \langle 0 | c_{I_1} \cdots c_{I_N} \, c_{n'}^\dagger c_n^\dagger c_m c_{m'} \, c_{I'_N}^\dagger \cdots c_{I'_1}^\dagger | 0 \rangle$$

normal-order and evaluate overlap (determinant)

orthonormal basis:

$$c_6^\dagger c_2 |\Phi_{I(181)}\rangle = c_6^\dagger c_2 \, c_7^\dagger c_5^\dagger c_4^\dagger c_2^\dagger c_0^\dagger |0\rangle$$

$$= (-1)^3 c_6^\dagger c_7^\dagger c_5^\dagger c_4^\dagger c_2 c_2^\dagger c_0^\dagger |0\rangle$$

$$= (-1)^3 c_6^\dagger c_7^\dagger c_5^\dagger c_4^\dagger \left(1 - c_2^\dagger c_2\right) c_0^\dagger |0\rangle$$

$$= (-1)^3 c_6^\dagger c_7^\dagger c_5^\dagger c_4^\dagger \cdot c_0^\dagger |0\rangle$$

$$= +|\Phi_{I(241)}\rangle = (-1)^2 c_7^\dagger c_6^\dagger c_5^\dagger c_4^\dagger \cdot c_0^\dagger |0\rangle$$

count set bits: `popcnt`

$$1\,0\,1\,1\,0\,1\,0\,1 \quad = \quad (-1)^c \;\; 1\,1\,1\,1\,0\,0\,0\,1$$

canonical NSA instruction

“Barcelona” Processor Feature: Advanced Bit Manipulation (ABM)

Posted by devcentral on September 26, 2007 in Processor Software Visible Features

One of the new instruction sets introduced in the Third Generation AMD Opteron™ processor is Advanced Bit Manipulation (ABM), comprising two instructions that operate on general purpose registers: LZCNT and POPCNT. We’ll first explore what POPCNT can do for you.

...

In addition to this specific scenario, there are several applications where pop count can substantially increase performance. Pop counts are used in cryptography (in fact, this instruction is also commonly called the ‘canonical NSA instruction’ because of the fact that the NSA refused to buy processors which didn’t support this instruction), encoding/decoding, databases (for quickly assessing information about data), and many others. One application that I find POPCNT most useful for is to quickly calculate Hamming distances. A Hamming distance is essentially a measure of how different one word is from another. Remember, this is not how different the values held by the words are (we could just use a subtract instruction to find that out!) but how the words themselves differ. For machine words, it is defined as the number of bits that are different between the two words.

http://developer.amd.com/community/blog/2007/09/26/barcelona-processor-feature-advanced-bit-manipulation-abm/

many-body problem

dimension of Hilbert space

ways of putting N electrons in K orbitals: $K\,(K–1)\,(K–2)\cdots(K–(N–1)) = K!/(K–N)!$

order in which electrons are put does not matter: $N!$

$$\dim \mathcal{H}_K^{(N)} = \frac{K!}{N!(K-N)!} = \binom{K}{N}$$

use symmetry to reduce dimension

e.g., spin conserved

$$\dim \mathcal{H}_{2K}^{(N_\uparrow,N_\downarrow)} = \binom{K}{N_\uparrow} \times \binom{K}{N_\downarrow}$$

```
>>> def binom(K,N):
...   if N==0:
...     return 1
...   else:
...     return (K-N+1)*binom(K,N-1)/N
...
>>> binom(24,12)**2
7312459672336
>>> binom(24,12)**2*8/2**30
54482
```

M	$N_\uparrow$	$N_\downarrow$	dimension of Hilbert space
2	1	1	4
4	2	2	36
6	3	3	400
8	4	4	4 900
10	5	5	63 504
12	6	6	853 776
14	7	7	11 778 624
16	8	8	165 636 900
18	9	9	2 363 904 400
20	10	10	34 134 779 536
22	11	11	497 634 306 624
24	12	12	7 312 459 672 336

sparseness

$$\langle \Phi_I | \hat{H} | \Phi_{I'} \rangle = \sum_{n,m} T_{nm} \langle 0 | c_{I_1} \cdots c_{I_N} \, c_n^\dagger c_m \, c_{I'_N}^\dagger \cdots c_{I'_1}^\dagger | 0 \rangle + \sum_{\substack{n'>n \\ m'>m}} \breve{U}_{nn',mm'} \langle 0 | c_{I_1} \cdots c_{I_N} \, c_{n'}^\dagger c_n^\dagger c_m c_{m'} \, c_{I'_N}^\dagger \cdots c_{I'_1}^\dagger | 0 \rangle$$

almost all matrix elements are zero, except

diagonal elements	1011001010	
single hop	1011100010	$N \times (K-N)$
pair-hop	1001100011	$N(N-1)/2 \times (K-N)(K-N-1)/2$

even more sparse for TB (short-range hopping)
and local Coulomb (Hubbard) interaction

matrix-vector products are *very* fast
classical simulations: Lanczos for low-energy states
finite basis set: high-energy states will be garbage…

Jordan-Wigner representations

First Quantization

Über quantentheoretische Umdeutung kinematischer und mechanischer Beziehungen.

Von **W. Heisenberg** in Göttingen

(Eingegangen am 29. Juli 1925.)

In der Arbeit soll versucht werden, Grundlagen zu gewinnen für die quantentheoretische Mechanik, die ausschließlich auf Beziehungen zwischen prinzipiell beobachtbaren Größen basiert ist.

Zeitschrift für Physik **33**, 879 (1925)

Sei $x(t)$ durch $\mathfrak{A}$, $y(t)$ durch $\mathfrak{b}$ charakterisiert, so ergibt sich als Darstellung von $x(t) \cdot y(t)$:

Klassisch:

$$\mathfrak{C}_\beta(n) = \sum_{-\infty}^{+\infty} \mathfrak{A}_\alpha(n)\mathfrak{B}_{\beta-\alpha}(n).$$

Quantentheoretisch:

$$\mathfrak{C}(n, n-\beta) = \sum_{-\infty}^{+\infty} \mathfrak{A}(n, n-\alpha)\mathfrak{B}(n-\alpha, n-\beta).$$

recognized as matrix multiplication in
M. Born and P. Jordan: Zur Quantenmechanik
Z. Phys. **34**, 858 (1925) (received 27 Sept)

$$\left[\hat{r}_x,\ \hat{p}_x\right] = \mathrm{i}\hbar$$

Second Quantization

The Quantum Theory of the Emission and Absorption of Radiation.

By P. A. M. Dirac, St. John's College, Cambridge, and Institute for Theoretical Physics, Copenhagen.

(Communicated by N. Bohr, For. Mem. R.S.—Received February 2, 1927.)

§1. *Introduction and Summary*

The new quantum theory, based on the assumption that the dynamical variables do not obey the commutative law of multiplication, has by now been developed sufficiently to form a fairly complete theory of dynamics. One can treat mathematically the problem of any dynamical system composed of a number of particles with instantaneous forces acting between them, provided it is describable by a Hamiltonian function, and one can interpret the mathematics physically by a quite definite general method. On the other hand, hardly anything has been done up to the present on quantum electrodynamics.

Proceedings of the Royal Society A **114**, 243 (1927)

$$\left[\hat{E},\ \hat{t}\right] = \mathrm{i}\hbar \quad \rightsquigarrow \quad E\,\mathrm{e}^{-\mathrm{i}\omega_n t} = \mathrm{e}^{-\mathrm{i}\omega_n t}\left(E + \hbar\omega_n\right)$$ (photon creator)

Lorentz invariance or $\hat{E} = \mathrm{i}\hbar\dfrac{d}{dt}$

Second Quantization

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§1. *Introduction and Summary*

$$\left[\hat{E},\ \hat{t}\right]=\mathrm{i}\hbar \ \rightsquigarrow\ E\,\mathrm{e}^{-\mathrm{i}\omega_n t}=\mathrm{e}^{-\mathrm{i}\omega_n t}\left(E+\hbar\omega_n\right)$$

(photon creator)

rewrite in terms of occupation numbers $N_k=\dfrac{E}{\hbar\omega_k}$ and phase $\theta_k=-\omega_k t$

number/phase uncertainty $[N, \theta] = -\mathrm{i}$

work with amplitudes of photon-field b_k

number of photons $N_k=\left|b_k\right|^2=b_k^\dagger b_k$

ansatz: $b_k=\mathrm{e}^{-\mathrm{i}\theta_k}N_k^{1/2}\ \left(b_k^\dagger=N_k^{1/2}\mathrm{e}^{+\mathrm{i}\theta_k}\right)\ \rightsquigarrow b_k^\dagger b_k=N_k$

$$\rightsquigarrow\ \left[b_k,\ b_k^\dagger\right]=\mathrm{e}^{-\mathrm{i}\theta_k}N_k\mathrm{e}^{\mathrm{i}\theta_k}-N_k=\mathrm{e}^{-\mathrm{i}\theta_k}\,\mathrm{e}^{\mathrm{i}\theta_k}(N_k+1)-N_k=1$$

Paulion operators

Zur Quantenmechanik der Gasentartung.

Von **P. Jordan** z. Z. in Kopenhagen

(Eingegangen am 7. Juli 1927.)

Von Dirac[1] ist kürzlich gezeigt worden, wie der Einsteinsche Gedanke, das ideale materielle Gas analog zum Lichtquantengas darzustellen durch gequantelte Wellen im gewöhnlichen dreidimensionalen Raume, quantenmechanisch exakt durchgeführt und mit der früher von Dirac[2] gegebenen, and die Schrödingersche Methode anknüfenden Darstellung (durch Eigenfunktionen in einem abstrakten Raume von zahllosen Dimensionen) in Verbindung gebracht werden kann. In dieser Arbeit wird eine entsprechende Theorie für das ideale Fermische statt Einsteinsche Gas entwickelt.

Pauli principle: N has eigenvalues 0 and 1

write as $N = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}(\sigma_z+1)$

corresponding ladder operator with $[N, \mathrm{e}^{\mathrm{i}\theta}] = \mathrm{e}^{\mathrm{i}\theta}$

$$\mathrm{e}^{\mathrm{i}\theta} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}(\sigma_x+\mathrm{i}\sigma_y)$$

creator $d^\dagger = N^{1/2}\mathrm{e}^{\mathrm{i}\theta} = \frac{1}{2}(\sigma_x+\mathrm{i}\sigma_y)$

$[d^\dagger, d]=\sigma_z$ canonical *anti*-commutation relation $\{d, d^\dagger\} = 1$

Z. Phys. **44**, 473 (1927)

Peierls:
limited uncertainty in N
⇒ no classical electron wave
(with well defined phase)

different modes commute:
hard-core bosons

Hard-Core Bosons

mapping to spin-$\frac{1}{2}$

$$S^{\pm} = S^x \pm \mathrm{i} S^y = (\sigma_x \pm \mathrm{i}\sigma_y)/2 \text{ and } S^z = \sigma_z/2$$

paulion	$\lvert 0 \rangle$	$\lvert 1 \rangle$	$d^\dagger$	d	N
spin-$\frac{1}{2}$	$\lvert \downarrow \rangle$	$\lvert \uparrow \rangle$	S^+	S^-	$S^z + \frac{1}{2}$

extend to multiple spins:

$$\{d_i,\, d_i^\dagger\} = 1 \quad \text{and} \quad \{d_i,\, d_i\} = 0 = \{d_i^\dagger,\, d_i^\dagger\}$$

while spin operators on different sites, $i \neq j$, commute

$$[d_i,\, d_j^\dagger] = 0 \quad \text{and} \quad [d_i,\, d_j] = 0 = [d_i^\dagger,\, d_j^\dagger]$$

hard-core bosons

problem: commutation relations not invariant under basis transforms...

e.g.: $d_\pm := (d_1 \pm d_2)/\sqrt{2} \rightsquigarrow [d_+,\, d_-] = N_2 - N_1 \neq 0$

makes solving spin models difficult

Fermion operators

Über das Paulische Äquivalenzverbot.

Von **P. Jordan** und **E. Wigner** in Göttingen

(Eingegangen am 26. Januar 1928.)

Die Arbeit enthält eine Fortsetzung der kürzlich von eimen der Verfasser vorgelegten Note "Zur Quantenmechanik der Gasentartung", deren Ergebnisse hier wesentlich erweitert werden. Es handelt sich darum, ein ideales oder nichtideales, dem Paulischen Äquivalenzverbot unterworfenes Gas zu beschreiben mit Begriffen, die keinen Bezug nehmen auf den abstrakten Koordinatenraum der Atomgesamtheit des Gases, sondern nur den gewöhnlichen dreidimensionalen Raum benutzen. Das wird ermöglicht durch die Darstellung des Gases vermittelst eines gequantelten dreidimensionalen Wellenfeldes, wobei die besonderen nichtkommutativen Multiplikationseigenschaften der Wellenamplitude gleichtzeitig für die Existenz korpuskularer Gasatome und für die Gültigkeit des Paulischen Äquivalenzverbots verantwortlich sind. Die Einzelheiten der Theorie besitzen enge Analogien zu der entsprechenden Theorie für Einsteinsche ideale oder nichtideale Gase, wie sie von Dirac, Klein und Jordan ausgeführt wurde.

Zeitschrift für Physik **47**, 631 (1928)

make algebra invariant under basis transforms: all operators must (anti)commute

Fermions

canonical anticommutation relations

$$\{c_i,\, c_j^\dagger\} = \delta_{ij} \quad \text{and} \quad \{c_i,\, c_j\} = 0 = \{c_i^\dagger,\, c_j^\dagger\}$$

invariant under basis transforms

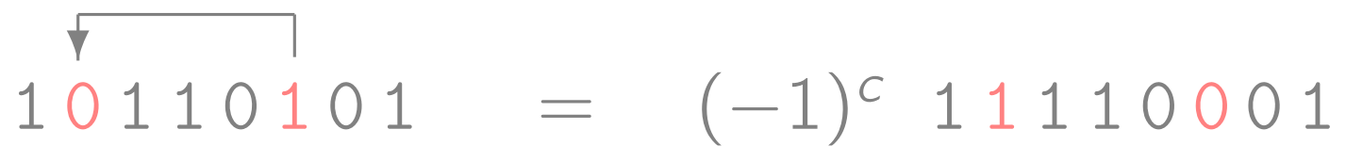
how to make operators on different modes anticommute?

$$c_i^\dagger := S_i^+ \otimes (-\sigma_{i-1}^z) \otimes \cdots \otimes (-\sigma_1^z)$$

with Fermi string operator $\prod_{k=1}^{i-1}(-\sigma_k^z)$

$$\text{e.g.: } \{c_i, c_i^\dagger\} = \{S_i^-, S_i^+\} \otimes \left(-\sigma_{i-1}^z\right)^2 \otimes \cdots \otimes \left(-\sigma_1^z\right)^2 = 1$$

$$\{c_i, c_j^\dagger\} = S_i^- \otimes \left(-\sigma_{i-1}^z\right) \otimes \cdots \left(-\sigma_{j+1}^z\right) \otimes \underbrace{\{S_j^+, -\sigma_i^z\}}_{=0} \otimes \left(-\sigma_{j-1}^z\right)^2 \otimes \cdots \left(-\sigma_1^z\right)^2 = 0$$



spin-½ models

direct mapping to hard-core bosons

$$S^x = (S^+ + S^-)/2 \;\rightarrow (d^\dagger + d)/2$$
$$S^y = (S^+ - S^-)/2\mathrm{i} \rightarrow (d^\dagger - d)/2\mathrm{i}$$
$$S^z \;\rightarrow\; d^\dagger d - \tfrac{1}{2}$$

$$J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j \quad \Leftrightarrow \quad J\sum_{\langle ij\rangle} \frac{1}{2}\left(d_i^\dagger d_j + d_i d_j^\dagger\right) + \left(d_i^\dagger d_i - \tfrac{1}{2}\right)\left(d_j^\dagger d_j - \tfrac{1}{2}\right)$$

hopping — Hubbard interaction

spin-rotation converts between 1- and 2-body terms

XY-models look easy (non-interacting hard-core bosons)
but: usual trick of diagonalizing 1-body matrix/Bogoliubov trafo does not work…

transform to fermions $\quad d_i^\dagger = c_i^\dagger \prod_{k=1}^{i-1} (-1)^{n_k}$

in general complicated non-local terms, *but*:
$d_i^\dagger d_i = c_i^\dagger c_i,\;\; d_{i+1}^\dagger d_i = c_{i+1}^\dagger c_i,\;\; d_{i+1}^\dagger d_i^\dagger = -c_{i+1}^\dagger c_i^\dagger$

solve spin-½ chains — Lieb, Schulz, Mattis, Ann. Phys. **16**, 411 (1968)

summary

indistinguishable electrons

$$\begin{vmatrix} \varphi_{\alpha_1}(x_1) & \varphi_{\alpha_2}(x_1) & \cdots & \varphi_{\alpha_N}(x_1) \\ \varphi_{\alpha_1}(x_2) & \varphi_{\alpha_2}(x_2) & \cdots & \varphi_{\alpha_N}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_{\alpha_1}(x_N) & \varphi_{\alpha_2}(x_N) & \cdots & \varphi_{\alpha_N}(x_N) \end{vmatrix}$$

(anti)symmetrization is hard
Slater determinants to the rescue

second quantization

$$= \left\langle 0 \middle| \hat{\psi}(x_1) \cdots \hat{\psi}(x_N)\; c^\dagger_{\alpha_N} \cdots c^\dagger_{\alpha_1} \middle| 0 \right\rangle$$

$$c_\alpha|0\rangle = 0 \qquad \{c_\alpha, c_\beta\} = 0 = \{c^\dagger_\alpha, c^\dagger_\beta\}$$

$$\langle 0|0\rangle = 1 \qquad \{c_\alpha, c^\dagger_\beta\} = \langle\alpha|\beta\rangle$$

antisymmetry guaranteed
operators independent of *N*

occupation number representation

$$|n_{K-1}, \ldots, n_0\rangle := \prod \left(c^\dagger_k\right)^{n_k} |0\rangle$$

bit counting

$$1\,0\,1\,1\,0\,1\,0\,1 = (-1)^c\; 1\,1\,1\,1\,0\,0\,0\,1$$

Jordan-Wigner mapping of spin-½

$$S^x = (S^+ + S^-)/2 \;\rightarrow (d^\dagger + d)/2$$
$$S^y = (S^+ - S^-)/2\mathrm{i} \rightarrow (d^\dagger - d)/2\mathrm{i}$$
$$S^z \;\rightarrow\; d^\dagger d - \tfrac{1}{2}$$

hard-core bosons
fermions with Fermi-string $\quad d^\dagger_i = c^\dagger_i \prod_{k=1}^{i-1} (-1)^{n_k}$

applications:

- solve (1d) spin models
- map fermions to Qbits
  exact diagonalization
  (still finite basis set…)