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Auxiliary-field quantum Monte Carlo calculations for the relativistic electron gas

M T Wilson and B L Gyorffy

H H Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK

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Abstract. We have written a version of the Hubbard–Stratonovich transformation for the case of the relativistic jellium, and have developed an auxiliary-field method for performing a quantum Monte Carlo calculation on such a system. We have successfully applied such a technique to a system with two electrons in a repeated box, and report on the results here. Also, we comment on the relationship between the functional form of the above theory and Feynman's formulation of quantum electrodynamics, namely the relationship of the auxiliary fields to the scalar and vector potentials in quantum electrodynamics. We find that gauge freedom enables us to find an auxiliary-field representation in which all fields are real, thus in principle removing the need to use imaginary auxiliary fields.

1. Introduction

The most generally useful and reliable first-principles method for studying the electronic structure of atoms, molecules and solids is density functional theory [1]. Used in conjunction with the local density approximation it is the only realistic way of proceeding to calculations involving large numbers of electrons. Performance of such calculations depends on knowledge of the energy of an homogeneous interacting electron gas (jellium) as a function of its density and magnetization, $E(n, m)$. For crystals containing heavy atoms, the electron density becomes very large around the nuclei, and relativistic effects become important.

Accurate exchange–correlation data are available for a non-relativistic jellium, due to the work of Ceperley and Alder [2]. However, their diffusion Monte Carlo (DMC) method relies on a mathematical trick—that is, exploiting the similarity between the Schrödinger equation and a diffusion equation. In the case of relativistic electrons, which obey the Dirac equation, no such similarity exists. Hence efforts to simulate relativistic electrons using the DMC method must rely on introducing relativistic corrections to the Schrödinger equation via perturbation theory. We are therefore lead into developing a new method which can deal with relativistic electrons exactly.

In auxiliary-field methods we decompose the many-body problem, via the Hubbard–Stratonovich transformation [5], into a one-body problem integrated over all possible external fields fluctuating in space and time. This allows us to use a range of one-body numerical techniques, as developed for one-body electronic structure calculations, to solve the problem numerically. The auxiliary-field method, like many others, uses the imaginary-time propagator to filter out the ground state of a Hamiltonian from a trial wavefunction $|\Phi\rangle$, that is,

$$\lim_{\beta\to\infty} \mathrm{e}^{-\beta\hat{H}}|\Phi\rangle = \langle\Psi_0|\Phi\rangle \mathrm{e}^{-\beta E_0}|\Psi_0\rangle \tag{1}$$

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where $|\Psi_0\rangle$ is the ground state of $\hat{H}$ with eigenvalue E_0. In principle $|\Phi\rangle$ can be chosen as *any* wavefunction not orthogonal to $|\Psi_0\rangle$.

The auxiliary-field method has been principally used in the study of the Hubbard Model and other short-range interaction models [3] but can also be applied to long-range interactions, notably the Coulomb interaction between electrons. Silvestrelli, Baroni and Car [4] have developed this method for such coulombic systems in the non-relativistic case. Such a method, being based on the Hubbard–Stratonovich transformation can be in principle developed for any two-body Hamiltonian. Thus this method is (in principle) able to cope with the interacting Dirac Hamiltonian as occurring in the relativistic jellium, and provides some hope for determining the $E(n, m)$ relation for densities where relativistic effects are important. The present work is a preliminary exploration of this possibility.

2. A relativistic many-body Hamiltonian for jellium

Throughout this paper we use a standard notation for relativistic quantum mechanics, that is:

$$\beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} \qquad \alpha = \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} \qquad \gamma^\mu = (\beta, \beta\alpha)$$

$$\sigma = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right).$$

We shall describe the relativistic jellium in a similar way to Ramana and Rajagopal [12] and MacDonald and Vosko [13], but leave out the interactions of electrons with free photons, to give an electron–electron interaction only, and ignore retardation effects. We write the time-independent Hamiltonian as

$$\hat{H} = \int_r \mathrm{d}^3 r \ \psi^\dagger(r)(-\mathrm{i}c\hbar\alpha \cdot \nabla + \beta mc^2)\psi(r) + \int_r \mathrm{d}^3 r \ \ ec\,\overline{\psi}(r)\gamma_\mu\psi(r)A^\mu_{\mathrm{rad}}(r) \tag{2}$$

where $\psi^\dagger(r)$ and $\psi(r)$ are four-component electron creation and annihilation operator fields respectively, $\overline{\psi}(r) = \psi^\dagger(r)\beta$, and $A^\mu_{\mathrm{rad}}(r)$ is the 4-potential describing the radiation field. The first term represents the kinetic part and the second term describes the interactions. The spin indices have been suppressed for clarity. Retardation effects have been removed by the introduction of time-independent wavefunctions.

The second term can be obtained by the following classical argument. We write the interaction between two electrons as

$$\hat{V}(r, t) = j_{1\mu}(r, t)A^\mu_{\mathrm{rad}}(r, t) \equiv \rho_1(r, t)\phi_{\mathrm{rad}}(r, t) - j_1(r, t) \cdot A_{\mathrm{rad}}(r, t) \tag{3}$$

where $j_1^\mu \equiv (\rho_1 c, j_1)$ is the 4-current due to electron 1 and $A^\mu_{\mathrm{rad}} \equiv (\phi_{\mathrm{rad}}/c, A_{\mathrm{rad}})$ is the 4-potential due to the presence of electron 2. This interaction is the simple sum of a charge–charge (Coulomb) term and a current–current (Breit) term. A detailed discussion of the origin of this interaction and the Breit term is given in [10]; in what follows we will end up using a static approximation to it. Recall that the Breit term tends to zero in the non-relativistic limit where one recovers the a description of the usual non-relativistic jellium. Note also the difference in sign between the two terms; this becomes important when performing the Hubbard–Stratonovich transformation below. In order to find A^μ_{rad}, we note that in the Lorentz gauge, Maxwell's equations can be written as

$$\Box_\nu \Box^\nu A^\mu_{\mathrm{rad}}(r, t) = \mu_0 j_2^\mu(r, t)$$

with the gauge constraint

$$\Box_\mu A^\mu_{\mathrm{rad}}(r, t) = 0 \tag{4}$$

where $\Box^\nu \equiv ((1/c)\,\partial/\partial t, -\nabla)$ is the 4-gradient. The solution to equation (4) is given by

$$A^\mu_{\rm rad}(r,t) = \frac{\mu_0}{4\pi}\int_{r'} {\rm d}^3r'\ \frac{j_2^\mu(r', t-|r-r'|/c)}{|r-r'|} + A^\mu_{\rm free}(r,t) \tag{5}$$

where $A^\mu_{\rm free}(r,t)$ is the complimentary function, so that $\Box_\nu\,\Box^\nu\,A^\nu_{\rm free}(r,t) = 0$, with the constraint $\Box_\mu A^\mu_{\rm free}(r,t) = 0$. These complimentary functions represent free photons and are ignored in the following derivation, so that we obtain an effective interaction between electrons only. However, they form an important part of quantum electrodynamics and so subtle quantum electrodynamic effects such as vacuum polarization are not treated here. We can now use the solution (5) to give us an effective electron–electron interaction;

$$\hat V(r,t) = \frac{\mu_0}{4\pi}\int_{r'} {\rm d}^3r'\ \frac{j_{1\mu}(r,t)\,j_2^\mu(r', t-|r-r'|/c)}{|r-r'|}. \tag{6}$$

We see that retardation is a relativistic effect and goes to zero in the non-relativistic limit. In order to be able to handle the Hamiltonian conveniently in the Hubbard–Stratonovich transformation we require that the two 4-currents be measured at the same time; thus we drop the retardation effect, and hence leave the pair interaction in this approximation as

$$\begin{aligned}\hat V(r,t) &= \frac{\mu_0}{4\pi}\int_{r'} {\rm d}^3r'\ \frac{j_{1\mu}(r,t)j_2^\mu(r',t)}{|r-r'|}\\ &\equiv \int_{r'} {\rm d}^3r'\ \overline{\phi}_1(r,t)\gamma_\mu\phi_1(r,t)\ v(r-r')\,\overline{\phi}_2(r',t)\gamma^\mu\phi_2(r',t)\end{aligned} \tag{7}$$

where $v(r-r') = e^2/4\pi\epsilon_0|r-r'|$ and $j_i^\mu(r,t) = ec\overline{\phi}_i(r,t)\gamma^\mu\phi_i(r,t)$. The effect of the retardation term is of order $\beta_{\rm F}^2$ (where $\beta_{\rm F} = \hbar k_{\rm F}/mc$), and so is of the same order in $\beta_{\rm F}$ as the leading corrections to the non-relativistic result due to relativity; hence, in general, it cannot be neglected. Nevertheless, in the present initial exploration of the theory we shall not deal with the extra complications its retention would involve. If we assume time independence in the wavefunctions, we can further write $\phi(r,t) = \phi(r)$ and so ignore all time-varying effects altogether.

Having obtained this effective pair interaction (7) we can now second quantize the interaction given in equation (2). Using $\psi(r) = \sum_i \phi_i(r)c_i$ and $\psi^\dagger(r) = \sum_i \phi_i^\dagger(r)c_i^\dagger$ we obtain the many-body Hamiltonian

$$\begin{aligned}\hat H = &\sum_{ij}\int_r {\rm d}^3r\ \overline{\phi}_i(r)(-{\rm i}c\hbar\gamma\cdot\nabla + mc^2)\phi_j(r)c_i^\dagger c_j\\ &+\frac{1}{2}\sum_{ijkl}\int_{rr'} {\rm d}^3r\ {\rm d}^3r'\ \overline{\phi}_i(r)\gamma_\mu\phi_k(r)v(r-r')\overline{\phi}_j(r')\gamma^\mu\phi_l(r')c_i^\dagger c_j^\dagger c_l c_k\end{aligned} \tag{8}$$

where the indices i, j, k, l contain both space and spin degrees of freedom implicitly. The interaction term is now exact if we consider a static distribution of charge. The Hamiltonian is of the required usual two-body form;

$$\hat H = \sum_{ij} T_{ij}c_i^\dagger c_j + \frac{1}{2}\sum_{ijkl} V_{ijkl}c_i^\dagger c_j^\dagger c_l c_k. \tag{9}$$

3. Hubbard–Stratonovich transformation (HST)

From here onwards, where there is no confusion, we will use the summation convention for summing over repeated indices. Central to our arguments is the well known [5] functional

integral representation of the density matrix:

$$e^{-\beta\hat{H}} = \int D\sigma_{ik}(t) \exp\left(\frac{1}{2}\int_{t=0}^{\beta} \sigma_{ik}(t) V_{ijkl} \sigma_{jl}(t)\ \mathrm{d}t\right) \times \exp\left(-\int_{t=0}^{\beta} (T_{ik} - V_{ijkl}\sigma_{jl}(t)) c_i^\dagger c_k\ \mathrm{d}t\right) \tag{10}$$

which reduces the two-body interaction to a one-body term at the expense of introducing time-dependent auxiliary fields $\sigma_{ik}(t)$ over which we must perform a functional integral. We have removed a self-energy term which cancels in all physical observables [7]. If $\hat{V}$ has no spin dependence, and is a central potential, the above expression reduces to

$$e^{-\beta\hat{H}} = \int D\sigma(r,t)\ \exp\left(\frac{1}{2}\int_{r,r'} \mathrm{d}^3r\ \mathrm{d}^3r'\ \int_{t=0}^{\beta} \sigma(r,t) v(r-r') \sigma(r',t)\ \mathrm{d}t\right) \times \exp\left(-\int_{t=0}^{\beta}\left[T(r,r')c_r^\dagger c_{r'} - \int_{r'} \mathrm{d}^3r'\ v(r-r')\sigma(r',t)c_r^\dagger c_r\right]\ \mathrm{d}t\right). \tag{11}$$

Depending on whether $\hat{V}$ is positive definite or negative definite, we must pick $\sigma(r,t)$ as pure imaginary or pure real respectively, so that the functional integral converges. To apply the propagator we must split the time-dependent evolution operator into time slices, and apply a kinetic and potential propagation at each time slice.

In order to use the above transformation we must choose an appropriate basis set for the $\phi_i(r,\xi)$ wavefunctions. It is natural to use the plane-wave Dirac spinors for the kinetic part and localized delta-function wavefunctions for the potential part. Thus we split the one-electron evolution operator of (10) into Trotter time slices of length $\Delta\tau$, in the form

$$\hat{U}(\sigma) = \hat{U}(\sigma_N)\cdots\hat{U}(\sigma_1) = \prod_{n=1}^{N} \exp\left(-T_{ik}c_i^\dagger c_k\,\Delta\tau\right)\exp\left(+V_{ijkl}\sigma_{jl}(n)c_i^\dagger c_k\,\Delta\tau\right) + \mathrm{O}(\Delta\tau^2) \tag{12}$$

where $N\,\Delta\tau = \beta$. We now introduce the basis sets.

For the kinetic part, we use the free Dirac spinors;

$$\phi_i(r) = \exp(\mathrm{i}k_i r)\begin{pmatrix} \chi^{(0)} \\ \{\hbar c\sigma k_i/(E_{k_i} + mc^2)\}\chi^{(0)} \end{pmatrix}\left(\frac{E_{k_i} + mc^2}{2mc^2}\right)^{1/2}$$

with

$$\chi^{(0)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ or } \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad E_{k_i}^2 = \hbar^2c^2k_i^2 + m^2c^4$$

and

$$\sigma = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right). \tag{13}$$

There are a total of four spin states possible. These are the free-electron spinors, solutions to the non-interacting Dirac problem. We have normalized the spinors covariantly, but for numerical calculations the normalization is, in fact, arbitrary.

Thus

$$T_{ij}a_i^\dagger a_j \equiv \sum_{i,s_i} \epsilon_{i,s_i} a_{i,s_i}^\dagger a_{i,s_i}$$

where

$$\epsilon_{i,s_i} = \pm(\hbar^2c^2k_i^2 + m^2c^4)^{1/2} \tag{14}$$

and so the kinetic term is diagonal. To avoid later confusion we replace c and $c^\dagger$ by a and $a^\dagger$ when we are dealing with the free-electron creation and annihilation operators, as in the kinetic energy case here.

For the potential part, consider the basis set

$$\phi_i(r,\xi) = \delta(r - r_i)\,\chi_{s_i}(\xi)$$

where

$$\chi_{s_i} \equiv \begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \begin{pmatrix}0\\0\\0\\1\end{pmatrix} \tag{15}$$

for $s_i = \uparrow, \downarrow, \overline{\uparrow}, \overline{\downarrow}$ respectively.

Substituting these into the expression for $\frac{1}{2}V_{ijkl}c_i^\dagger c_j^\dagger c_l c_k$ from equations (8) and (9), we obtain:

$$\hat{V} = \frac{1}{2}\int_{rr'} \mathrm{d}^3r\ \mathrm{d}^3r'\ v(r-r')M_{s_is_ks_js_l}c_{s_i}^\dagger(r)c_{s_k}(r)c_{s_j}^\dagger(r')c_{s_l}(r')$$

where

$$\begin{aligned} M_{s_is_ks_js_l} &\equiv \sum_{\xi_i\xi_k}\chi_{s_i}^*(\xi_i)\beta\gamma_\mu(\xi_i,\xi_k)\chi_{s_k}(\xi_k)\sum_{\xi_j\xi_l}\chi_{s_j}^*(\xi_j)\beta\gamma^\mu(\xi_j,\xi_l)\chi_{s_l}(\xi_l) \\ &= \overline{\chi}_{s_i}\gamma_\mu\chi_{s_k}\overline{\chi}_{s_j}\gamma^\mu\chi_{s_l}. \end{aligned} \tag{16}$$

Most of the elements $M_{s_is_ks_js_l}$ are zero. Making the following definitions:

$$\begin{aligned} \hat{\rho}_c(r) &= c_\uparrow^\dagger(r)c_\uparrow(r) + c_\downarrow^\dagger(r)c_\downarrow(r) + c_{\overline{\uparrow}}^\dagger(r)c_{\overline{\uparrow}}(r) + c_{\overline{\downarrow}}^\dagger(r)c_{\overline{\downarrow}}(r) \\ \hat{\rho}_z(r) &= c_\uparrow^\dagger(r)c_{\overline{\uparrow}}(r) + c_{\overline{\uparrow}}^\dagger(r)c_\uparrow(r) - c_\downarrow^\dagger(r)c_{\overline{\downarrow}}(r) - c_{\overline{\downarrow}}^\dagger(r)c_\downarrow(r) \\ \hat{\rho}_x(r) &= c_\uparrow^\dagger(r)c_{\overline{\downarrow}}(r) + c_{\overline{\uparrow}}^\dagger(r)c_\downarrow(r) + c_\downarrow^\dagger(r)c_{\overline{\uparrow}}(r) + c_{\overline{\downarrow}}^\dagger(r)c_\uparrow(r) \\ \hat{\rho}_y(r) &= c_\uparrow^\dagger(r)c_{\overline{\downarrow}}(r) + c_{\overline{\uparrow}}^\dagger(r)c_\downarrow(r) - c_\downarrow^\dagger(r)c_{\overline{\uparrow}}(r) - c_{\overline{\downarrow}}^\dagger(r)c_\uparrow(r) \end{aligned} \tag{17}$$

and using the representation

$$\gamma^0 = \begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix} \qquad \gamma^1 = \begin{pmatrix}0&0&0&1\\0&0&1&0\\0&-1&0&0\\-1&0&0&0\end{pmatrix}$$

$$\gamma^2 = \begin{pmatrix}0&0&0&-\mathrm{i}\\0&0&\mathrm{i}&0\\0&\mathrm{i}&0&0\\-\mathrm{i}&0&0&0\end{pmatrix} \qquad \gamma^3 = \begin{pmatrix}0&0&1&0\\0&0&0&-1\\-1&0&0&0\\0&1&0&0\end{pmatrix}$$

we find that we can can rewrite what remains in equation (16) as

$$\begin{aligned} \hat{V} = \frac{1}{2}\int_{rr'} \mathrm{d}^3r\ \mathrm{d}^3r'\ [&+\hat{\rho}_c(r)v(r-r')\hat{\rho}_c(r') - \hat{\rho}_x(r)v(r-r')\hat{\rho}_x(r') \\ &+\hat{\rho}_y(r)v(r-r')\hat{\rho}_y(r') - \hat{\rho}_z(r)v(r-r')\hat{\rho}_z(r')]. \end{aligned} \tag{18}$$

The point of these transformations is that the above form enables us to perform a HST as defined in equation (11) on each of the four parts of the potential, as follows.

We introduce a separate auxiliary field $\sigma(r)$ to couple to each $\hat{\rho}$. For convergence of the functional integral we must use an imaginary version of the HST for $\hat{\rho}_c$ and $\hat{\rho}_y$, but a real HST for $\hat{\rho}_x$ and $\hat{\rho}_z$. Putting all this together using equations (11), (12), (14) and (18), we obtain the functional integral

$$e^{-\beta\hat{H}} = \int \mathrm{D}\sigma_c\,\mathrm{D}\sigma_x\,\mathrm{D}\sigma_y\,\mathrm{D}\sigma_z\; G(\sigma_c)G(\sigma_x)G(\sigma_y)G(\sigma_z)\prod_{t=1}^{N}\exp\left(-\Delta\tau\left(\epsilon_{i,s_i}a^{\dagger}_{i,s_i}a_{i,s_i}\right)\right)$$
$$\times\exp\left[-\Delta\tau\left(\mathrm{i}v\sigma_c(t)\hat{\rho}_c - v\sigma_x(t)\hat{\rho}_x + \mathrm{i}v\sigma_y(t)\hat{\rho}_y - v\sigma_z(t)\hat{\rho}_z\right)\right]$$

where we have suppressed all integrals where possible and used the notation

$$v\sigma_i(t)\hat{\rho}_i \equiv \int_{rr'} \mathrm{d}^3r\;\mathrm{d}^3r'\; v(r-r')\sigma_i(r',t)\hat{\rho}_i(r)$$

and

$$G(\sigma_i) \equiv \exp\left(-\frac{1}{2}\int_{rr'}\mathrm{d}^3r\;\mathrm{d}^3r'\;\int_{t=0}^{\beta}\sigma_i(r,t)v(r-r')\sigma_i(r',t)\;\mathrm{d}t\right). \tag{19}$$

4. Interpretation of the auxiliary fields

The auxiliary fields which appear in Hubbard–Stratonovich transformations are purely mathematical constructions whose sole role is to facilitate a convenient integral represenation of operator functions. In what follows we show that the above four fields are closely related to the electromagnetic fields generated by the moving charges of the model.

Writing out a single time slice of the potential part of the one-electron propagator using equations (17) and (19) gives us

$$\hat{U}_V(\sigma_c,\sigma_x,\sigma_y,\sigma_z) = \exp\left(-\Delta\tau\,(v\sigma)_{s_is_k}(r)c^{\dagger}_{s_i}c_{s_k}(r)\right)$$

where

$$(v\sigma)(r) \equiv \begin{pmatrix} \mathrm{i}v\sigma_c & 0 & -v\sigma_z & -v\sigma_x+\mathrm{i}v\sigma_y \\ 0 & \mathrm{i}v\sigma_c & -v\sigma_x-\mathrm{i}v\sigma_y & v\sigma_z \\ -v\sigma_z & -v\sigma_x+\mathrm{i}v\sigma_y & \mathrm{i}v\sigma_c & 0 \\ -v\sigma_x-\mathrm{i}v\sigma_y & v\sigma_z & 0 & \mathrm{i}v\sigma_c \end{pmatrix}. \tag{20}$$

We see that this is simply

$$\exp\left(-\Delta\tau\left(\mathrm{i}v\sigma_c I_{s_is_k} - \alpha_{s_is_k}\cdot v\boldsymbol{\sigma}\right)c^{\dagger}_{s_i}c_{s_k}\right) \tag{21}$$

where $v\boldsymbol{\sigma} = (v\sigma_x, v\sigma_y, v\sigma_z)$. We can now compare this to a single-particle Dirac Hamiltonian $\hat{H}_D$ in the presence of scalar and vector potentials. Writing

$$\hat{H}_D = (-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\nabla + \beta mc^2 - ec\boldsymbol{\alpha}\cdot A + e\phi)$$

gives us

$$\exp(-\Delta\tau\,\hat{H}_D) = \exp(-(-\mathrm{i}c\hbar\boldsymbol{\alpha}\cdot\nabla + \beta mc^2)\Delta\tau)\exp(-(e\phi I - ec\boldsymbol{\alpha}\cdot A)\Delta\tau). \tag{22}$$

Hence we can immediately see the interpretation of the external fields as fields due to the scalar and vector potentials. The first term in equation (21) is the straightforward Coulomb propagation in an imaginary field. We see that $v\sigma_c$ represents a scalar potential, $e\phi(r,t)$. The second term is a 'current' propagation, and the components of the field $v\boldsymbol{\sigma}$ represent components of a vector potential (times the speed of light,) $ecA(r,t)$. Thus we have recovered a term in the propagator of similar form to $j_\mu A^\mu$, albeit with the scalar potential having an imaginary value. The presence of this imaginary field can be traced back to the

relativistic metric; normally the Coulomb part enters with the opposite sign to the Breit part. Thus this representation suffers from the fact that the single-time-step propagator $\hat{U}(\sigma_k)$ is *not* a Hermitian operator, and so in general we are not able to apply the techniques of Hermitian matrices.

Prompted by the above observation we are lead to an attempt to interpret the argument of the gaussian weight as the energy of free fields. To do this we note that the gaussian weight term $G(\sigma_c)$ looks like

$$-\frac{1}{2}\sigma_c v\sigma_c \equiv -\frac{1}{2}\int_{rr'} d^3r\ d^3r' \int_{t=0}^{\beta} \sigma_c(r,t)v(r-r')\sigma_c(r',t)\ dt$$

which can be written as

$$-\frac{1}{2}\sigma_c v\sigma_c \equiv -\int_{t=0}^{\beta} v\sigma_c(s;t)v^{-1}(s,s')v\sigma_c(s',t)\ dt \tag{23}$$

where $v\sigma_c(s,t)$ is defined as in equation (19) and $v^{-1}(s,s')$ is the inverse operator of $v(s,s')$. Now, considering the identity

$$\nabla_r^2 v(r-r') \equiv \nabla_r^2\left(\frac{e^2}{4\pi\epsilon_0|r-r'|}\right) \equiv -\frac{e^2}{\epsilon_0}\delta^3(r-r') \tag{24}$$

we have

$$v(r) \equiv -\frac{e^2}{\epsilon_0}\nabla_r^{-2} \qquad \text{or} \qquad v^{-1}(r) \equiv -\frac{\epsilon_0}{e^2}\nabla_r^2. \tag{25}$$

Writing the argument of the gaussian weight as in equation (23) we see that schematically it is of the form

$$-\frac{1}{2}\sigma_c v\sigma_c = -\frac{1}{2}v\sigma_c\left(\frac{-\epsilon_0}{e^2}\right)\nabla_r^2 v\sigma_c \tag{26}$$

which on integrating by parts may be rewritten as

$$\frac{1}{2}\sigma_c v\sigma_c = \frac{\epsilon_0}{2e^2}|\nabla_r(v\sigma_c)|^2. \tag{27}$$

Thus by putting $iv\sigma_c \equiv e\phi$ we see that this is just the $-(\epsilon_0/2)|\nabla_r\phi|^2$ term that appears in the quantum electrodynamics (QED) expression below.

Recall now that in the Lorentz gauge the Feynman formulation of the QED expression for the term $\exp((i/\hbar)\int L\,d^3r\ dt)$, where L is the Lagrangian density, is given by [6]

$$\begin{aligned} S &= \exp\left((i/\hbar)\int L\,d^3r\ dt\right) \\ &= \int D\phi\ DA\ \exp\left(\frac{i}{\hbar}\int_{t=0}^{T} dt\ \frac{\epsilon_0}{2}\left[+|\nabla\phi|^2 + \dot{A}^2 - \left(\frac{\dot{\phi}}{c}\right)^2\right.\right. \\ &\quad \left.\left. -c^2\sum_{ij}\left(\frac{\partial A_j}{\partial x_i}\right)^2\right] - \rho\phi + j\cdot A\right). \end{aligned} \tag{28}$$

Performing a Wick rotation to imaginary time, ($iT/\hbar = \beta$, $it/\hbar = \tau$) we obtain

$$\begin{aligned} Z &= \exp(-\beta\hat{H}) \\ &= \int D\phi\ DA\ \exp\left(\int_{\tau=0}^{\beta} d\tau\ \frac{\epsilon_0}{2}\left[-|\nabla\phi|^2 - \dot{A}^2 - \left(\frac{\dot{\phi}}{c}\right)^2\right.\right. \\ &\quad \left.\left. -c^2\sum_{ij}\left(\frac{\partial A_j}{\partial x_i}\right)^2\right] - i\rho\phi + j\cdot A\right) \end{aligned} \tag{29}$$

where the 'i' comes from making the scalar potential ϕ imaginary in order to make the integral converge. We thus see the direct similarity between the one-electron propagator term in the HST (20) and the $j \cdot A - i\rho\phi$ term in QED, and the gaussian term in the HST and the $(\epsilon_0/2)|\nabla\phi|^2$ term in QED. We note however that the HST produces no terms equivalent to the $\dot{\phi}$ and $\dot{A}$ terms that are present in the QED formulation. Clearly this is the consequence of neglecting the effects of retardation. Although our Hamiltonian does not contain effects such as vacuum polarization, we see that nonetheless the HST gives very similar physics to QED. It is likely that if effects such as retardation and free photons are included in our Hamiltonian (8) then full QED could be recovered. However, numerical work with such a functional representation would not be so straight forward, so this possibility has not been explored.

It is easy to show that making the time-independent saddle point approximation to the functional integral in equation (19) yields the relativistic analogue to the Hartree equations—that is, the self-consistent set of single-particle Dirac equations

$$(-ic\hbar\alpha \cdot \nabla + \beta mc^2 + e\phi - ec\alpha \cdot A)\phi_k = \varepsilon^{(k)}\phi_k$$

where the 4-potential is given by

$$A^\mu(r) \equiv (\phi(r)/c, A(r)) = \frac{\mu_0 ec}{4\pi} \sum_{i=1}^{N} \int_{r'} d^3r' \; \frac{\overline{\phi}_i(r')\gamma^\mu \phi_i(r')}{|r - r'|}. \tag{30}$$

Also, we find that by considering second-order fluctuations about the saddle point of the functional integral we obtain the relativistic equivalent of the random phase approximation (RPA), in an exactly analogous way tothat followed in the non-relativistic case [14].

Having identified the auxiliary fields with the scalar and vector potentials, we see that there is a natural way to add in the effects of external potentials $\phi^{ext}(r)$ and $A^{ext}(r)$, by simply adding $e\phi^{ext}(r)$ to $iv\sigma_c(r, t)$ and $ecA^{ext}(r)$ to $v\sigma(r, t)$ in the one-electron propagator.

5. Monte Carlo calculation of ground state energy

Non-relativistically, following Sugiyama and Koonin [7], we use the usual projection operator $e^{-\beta\hat{H}}$ and operate it on a trial wavefunction $|\Phi\rangle$. Then it is easy to show that

$$E_0 = \lim_{\beta\to\infty} E(\beta) = \lim_{\beta\to\infty} \frac{\langle\Phi|\hat{H}e^{-\beta\hat{H}}|\Phi\rangle}{\langle\Phi|e^{-\beta\hat{H}}|\Phi\rangle}. \tag{31}$$

We must adapt this relativistically, because of the presence of negative energy states. Thus we consider the operation $\hat{P}(e^{-\beta\hat{H}})$, where the $\hat{P}$-operator removes all negative energy states. This is equivalent to requiring that all negative energy states remain filled. Then,

$$E_0 = \lim_{\beta\to\infty} E(\beta) = \lim_{\beta\to\infty} \frac{\langle\Phi|\hat{H}\hat{P}e^{-\beta\hat{H}}|\Phi\rangle}{\langle\Phi|\hat{P}e^{-\beta\hat{H}}|\Phi\rangle}. \tag{32}$$

Potentially there is a numerical problem here, since as β increases the negative energy states will grow and swamp the positive ones in which we are interested. However, in our calculations we find that we can still extract the positive states without problem. For the numerical simulations, it is in fact more convenient to consider a symmetric form of (32), that is,

$$E_0 = \lim_{\beta\to\infty} E(\beta) = \lim_{\beta\to\infty} \frac{\langle\Phi|e^{-(\beta/2)\hat{H}}\hat{P}^\dagger\hat{H}\hat{P}e^{-(\beta/2)\hat{H}}|\Phi\rangle}{\langle\Phi|\hat{P}e^{-\beta\hat{H}}|\Phi\rangle} \tag{33}$$

and operate the time evolution operator for time $\beta/2$ on each side of the determinant.

We can now apply the relativistic HST as in equation (19). This gives us a one-electron problem with four auxiliary fields. We choose as a trial determinant an antisymmetric combination of solutions of the free Dirac equation, given by (13). To propagate these, we perform the kinentic energy part of the propagation in reciprocal space, and the potential energy part in real space. We can move between the two bases easily by the fast Fourier transform. The kinetic part is simple—we just write every one-electron wavefunction as a sum of solutions of the free Dirac equation, and propagate each by its eigenvalue before combining them back together. To do the potential part, we need to be able to deal with the matrix $v\sigma(r)$ in equation (20) at every point in real space. To do this we split it into its anti-Hermitian and Hermitian parts:

$$\begin{aligned}(v\sigma)(r) &\equiv \begin{pmatrix} \mathrm{i}v\sigma_c & 0 & -v\sigma_z & -v\sigma_x+\mathrm{i}v\sigma_y \\ 0 & \mathrm{i}v\sigma_c & -v\sigma_x-\mathrm{i}v\sigma_y & v\sigma_z \\ -v\sigma_z & -v\sigma_x+\mathrm{i}v\sigma_y & \mathrm{i}v\sigma_c & 0 \\ -v\sigma_x-\mathrm{i}v\sigma_y & v\sigma_z & 0 & \mathrm{i}v\sigma_c \end{pmatrix} \\ &\equiv \begin{pmatrix} \mathrm{i}v\sigma_c & 0 & 0 & 0 \\ 0 & \mathrm{i}v\sigma_c & 0 & 0 \\ 0 & 0 & \mathrm{i}v\sigma_c & 0 \\ 0 & 0 & 0 & \mathrm{i}v\sigma_c \end{pmatrix} \\ &\quad - \begin{pmatrix} 0 & 0 & v\sigma_z & v\sigma_x-\mathrm{i}v\sigma_y \\ 0 & 0 & v\sigma_x+\mathrm{i}v\sigma_y & -v\sigma_z \\ v\sigma_z & v\sigma_x-\mathrm{i}v\sigma_y & 0 & 0 \\ v\sigma_x+\mathrm{i}v\sigma_y & -v\sigma_z & 0 & 0 \end{pmatrix}. \end{aligned} \tag{34}$$

The first (anti-Hermitian) part is simple to propagate with, since it is diagonal. This part is equivalent to the usual imaginary-field propagation in the non-relativistic method of Silvestrelli, Baroni and Car [4]. The second (Hermitian) part is more difficult; to perform it we need to know the eigenstates of the Hermitian matrix in equation (34).

Writing $q_i \equiv v\sigma_i$ and $|q| \equiv \left(q_x^2+q_y^2+q_z^2\right)^{1/2}$, we find that the normalized eigenvectors of the Hermitian part of equation (34) are given by

$$u_1 = \frac{1}{2(|q|^2-q_z|q|)^{1/2}} \begin{pmatrix} -q_x+\mathrm{i}q_y \\ q_z-|q| \\ -q_x+\mathrm{i}q_y \\ q_z-|q| \end{pmatrix} \qquad u_2 = \frac{1}{2(|q|^2-q_z|q|)^{1/2}} \begin{pmatrix} -q_x+\mathrm{i}q_y \\ q_z-|q| \\ q_x-\mathrm{i}q_y \\ -q_z+|q| \end{pmatrix}$$

$$u_3 = \frac{1}{2(|q|^2+q_z|q|)^{1/2}} \begin{pmatrix} -q_x+\mathrm{i}q_y \\ q_z+|q| \\ -q_x+\mathrm{i}q_y \\ q_z+|q| \end{pmatrix} \qquad u_4 = \frac{1}{2(|q|^2+q_z|q|)^{1/2}} \begin{pmatrix} -q_x+\mathrm{i}q_y \\ q_z+|q| \\ q_x-\mathrm{i}q_y \\ -q_z-|q| \end{pmatrix} \tag{35}$$

with the corresponding eigenvalues $\varepsilon_1 = \varepsilon_4 = +|q|$, $\varepsilon_2 = \varepsilon_3 = -|q|$. Hence we can perform the Breit (Hermitian) part of the propagation by writing the four-component wavefunction at every point in space in terms of these eigenvectors, and propagating with the corresponding eigenvalue.

For sampling the auxiliary σ-fields we use a technique similar to that of Silvestrelli *et al* [4]. Defining $\hat{U}(\sigma)$ by equation (12), $G(\sigma_i)$ by equation (19) and writing $G(\sigma) =$

$G(\sigma_c)G(\sigma_x)G(\sigma_y)G(\sigma_z)$ we write

$$D(\sigma) = \mathrm{Re}\langle\Phi|\hat{U}_{\beta/2\to\beta}(\sigma)\hat{P}^\dagger\hat{P}\hat{U}_{0\to\beta/2}(\sigma)|\Phi\rangle$$
$$E(\sigma) = \frac{\mathrm{Re}\langle\Phi|\hat{U}_{\beta/2\to\beta}\hat{P}^\dagger\hat{H}\ \hat{P}\hat{U}_{0\to\beta/2}(\sigma)|\Phi\rangle}{\mathrm{Re}\langle\Phi|\hat{U}_{\beta/2\to\beta}(\sigma)\hat{P}^\dagger\hat{P}\hat{U}_{0\to\beta/2}(\sigma)|\Phi\rangle} \tag{36}$$
$$S(\sigma) = \frac{D(\sigma)}{|D(\sigma)|}$$

where we also have removed the negative energy states as in equation (33). Applying the HST to $e^{-\beta\hat{H}}$ as given in equation (19) and substituting in (33) gives us

$$E_0 = \lim_{\beta\to\infty}\left[\left(\int \mathrm{D}\sigma\ G(\sigma)\ |D(\sigma)|\ E(\sigma)S(\sigma)\right) \Big/ \left(\int \mathrm{D}\sigma\ G(\sigma)\ |D(\sigma)|\ S(\sigma)\right)\right]. \tag{37}$$

We see that from (37) we can now apply a Metropolis technique [8] to evaluate this ratio, where the probability distribution is given by $G(\sigma)|D(\sigma)|$. We have the usual auxiliary-field sign problem, since if $\langle S(\sigma)\rangle \approx 0$, when we average in the $G(\sigma)|D(\sigma)|$ probability distribution the value of E_0 will have a large statistical error.

We pick σ-fields from the gaussian distribution by using the Box–Müller method [14]. We then can propagate the trial determinant by these fields as in equations (12) and (19) in order to find $D(\sigma)$, and carry out a Metropolis ratio test on $|D(\sigma)|$ so that we successfully sample the probability distribution $p(\sigma) = G(\sigma)|D(\sigma)|$.

As matters of technical details we record that we use periodic boundary conditions on a box of length L ($\Omega = L^3$) and expand everything in terms of its Fourier components. Thus, the $1/r$-potential for jellium becomes inside the box

$$v(r-r') = \frac{e^2}{4\pi\epsilon_0}\sum_{g\neq 0}\frac{4\pi}{\Omega g^2}e^{ig(r-r')}$$

where

$$g = \frac{2\pi}{L}(n_x, n_y, n_z) \qquad n_x, n_y, n_z \in \mathbb{Z} \tag{38}$$

and we sum over all Fourier components except the constant ($g = 0$) term, since this is removed by the positive background in jellium. We impose a cut-off in the numbers of Fourier components considered; in the case of the following calculations we have used 27 ($= 3^3$), 125 ($= 5^3$) or 343 ($= 7^3$) components.

Calculations were performed on a CRAY Y-MP8 supercomputer. However, the heavy computational workload means that we are limited to small numbers of electrons—in this case two only (one spin 'up', the other spin 'down').

For the numerical calculations we have used atomic units (au) chosen such that

$$\frac{\hbar^2}{m} = 1 \qquad \frac{e^2}{4\pi\epsilon_0} = 1 \qquad c = 1$$

so that

$$a_0 = \frac{\hbar^2}{me^2}(4\pi\epsilon_0) = 1 \qquad R_\infty = \frac{m}{2\hbar^2}\frac{e^4}{(4\pi\epsilon_0)^2} = \frac{1}{2}$$

where a_0 and R_∞ are the Bohr radius and Rydberg constant respectively.

We have illustrated the method with a calculation for a two-electron repeated jellium system at a density of $r_s = 0.0140$ au where r_s is given by the radius of the sphere that on average contains one electron, that is $\frac{4}{3}\pi r_s^3 = \Omega/N$. Such an electron density has a

Fermi velocity corresponding to $\beta_F = v_F/c = \hbar k_F/mc = 1$ so is well into the relativistic régime. We have chosen to consider up to 343 Fourier components for the wavefunctions and σ-fields, and have used Trotter time slices of length 2.5×10^{-6} au and 5×10^{-6} au. We have chosen a trial wavefunction of an 'up' and a 'down' electron situated at the Γ point in reciprocal space. We have carried out calculations for both the non-relativistic and relativistic jellium. The results are presented below in figures 1 and 2 for the basis sets of 343 and 125 plane waves respectively, in the form of a plot of energy per particle (minus rest-mass energy) as given by equation (33) against β. In these figures it is easy to see the extent of the statistical error. In fact this error is almost entirely due to the fluctuations in $E(\sigma)$ as defined in equation (36) since the average sign is very close to 1 for the whole range of β used.

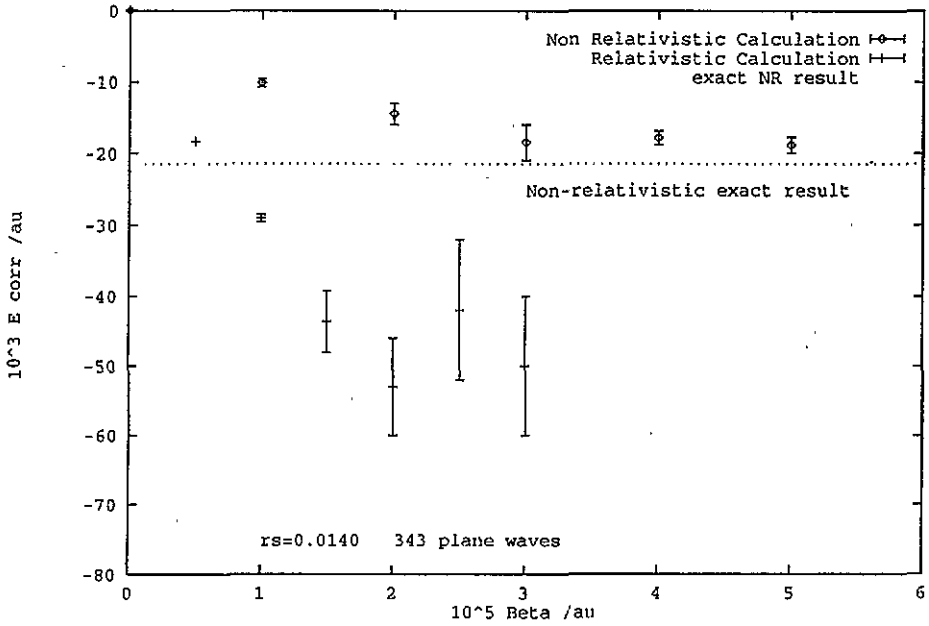

Figure 1. AFQMC calculations of correlation energy E_c against β for a two-electron system at density $r_s = 0.0140$, using a basis set of 343 plane waves. The 4-field representation of equation (19) is used for the relativistic case, and the 1-field representation in equation (11) is used for the non-relativistic case. $\Delta\tau = 2.5 \times 10^{-6}$ for the relativistic case, and $\Delta\tau = 5.0 \times 10^{-6}$ for the non-relativistic case.

In order to interpret our results we should like to be able to compare the relativistic correlation energy with the non-relativistic correlation energy at the same value of r_s. In the case of two non-relativistic electrons, we are able to solve the Schrödinger equation numerically by writing

$$\left(-\frac{\hbar^2}{2m}\nabla_{r_1}^2 - \frac{\hbar^2}{2m}\nabla_{r_2}^2 + v(r_1 - r_2)\right)\Psi(r_1, r_2) = E\Psi(r_1, r_2) \tag{39}$$

and making the standard substitution $R = r_1 + r_2, r = r_1 - r_2, \Psi(r_1, r_2) = \Phi(R)\phi(r)$ to give

$$\left(-\frac{\hbar^2}{2m}(2\nabla_R^2) - \frac{\hbar^2}{2m}(2\nabla_r^2) + v(r)\right)\Phi(R)\phi(r) = E\Phi(R)\phi(r) \tag{40}$$

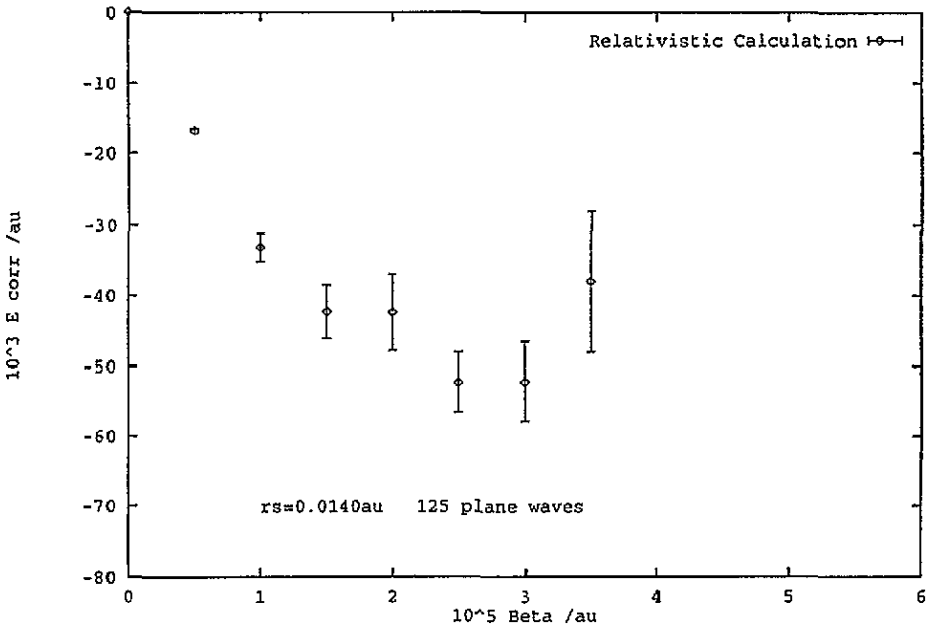

Figure 2. Relativistic AFQMC calculations of correlation energy E_c against β for a two-electron system at density $r_s = 0.0140$, using a basis set of 125 plane waves and the 4-field representation in equation (19). $\Delta\tau = 2.5 \times 10^{-6}$.

which is now separable. Numerical calculation of the solution to the r-part of this equation leads to the 'exact' non-relativistic result. In figure 1 we show the exact result as calculated in this way for $r_s = 0.0140$ au, and also an equivalent non-relativistic auxiliary-field quantum Monte Carlo calculation using the technique of Silvestrelli *et al* [4], for a basis set containing 343 plane waves. Unfortunately, such separation of variables does not occur in the case of the Dirac equation and hence we only have our Monte Carlo results to rely on.

6. Exploiting gauge freedom

Having identified the auxiliary fields with the scalar and vector potentials, we can exploit gauge freedom to find a new representation, in particular one in which the auxiliary fields are real.

In the propagator $\hat{U}(\sigma)$, as defined in equations (12) and (19), the effect of $iv\sigma_c(r,t)$ is identical to that of a scalar potential $e\phi(r,t)$, and that of the field $v\boldsymbol{\sigma}(r,t) = (v\sigma_x(r,t), v\sigma_y(r,t), v\sigma_z(r,t))$ is identical to that of a vector potential $ec\boldsymbol{A}(r,t)$. Hence we can choose another scalar and vector potential pair which give rise to the same $\boldsymbol{E}$- and $\boldsymbol{B}$-fields and so will have an identical effect in the real-time calculation of the wavefunction. In general, we can write such a gauge transformation as

$$\phi^{\text{new}} = \phi^{\text{old}} - \frac{\partial \chi}{\partial t} \qquad \boldsymbol{A}^{\text{new}} = \boldsymbol{A}^{\text{old}} + \nabla\chi \tag{41}$$

where $\chi(r,t)$ is *any* scalar function in space and time. This allows us to make the choice

$$\chi(r,t) = \int_{t'=0}^{t} \phi^{\text{old}}(r,t')\,\mathrm{d}t'$$

so that

$$\phi^{\text{new}}(r,t)=0 \qquad A^{\text{new}}(r,t)=A^{\text{old}}(r,t)+\int_{t'=0}^{t}\nabla\phi^{\text{old}}(r,t')\,\mathrm{d}t'. \tag{42}$$

Hence we have eliminated the scalar potential term in the propagator, in favour of an addition to the vector potential. It is important to realize that t in the above is *real* time. To find the representation in imaginary time (i.e. the density matrix) of $\exp(-\mathrm{i}\hat{H}T/\hbar)$ we must perform a Wick rotation, that is $\beta=\mathrm{i}T/\hbar$, $\tau=\mathrm{i}t/\hbar$. Thus $\partial/\partial t=(\partial\tau/\partial t)\,\partial/\partial\tau=(\mathrm{i}/\hbar)\,\partial/\partial\tau$ in imaginary time and so

$$\phi^{\text{new}}(r,\tau)=\phi^{\text{old}}(r,\tau)-\frac{\mathrm{i}}{\hbar}\frac{\partial\chi(r,\tau)}{\partial\tau} \qquad A^{\text{new}}(r,\tau)=A^{\text{old}}(r,\tau)+\nabla\chi(r,\tau). \tag{43}$$

Hence eliminating an *imaginary* ϕ in the imaginary time propagator requires a *real* $\chi(r,\tau)$, and so leads to a *real* A^{new}. Thus we are able to find a representation which uses real fields only.

Formally, we write the real-time evolution operator as

$$\exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}T\right)=\exp\left(-\frac{\mathrm{i}}{\hbar}\int_{t=0}^{T}\left(\hat{T}+\frac{1}{2}\left[\hat{\rho}_{\mathrm{c}}v\hat{\rho}_{\mathrm{c}}-\hat{\rho}_x v\hat{\rho}_x+\hat{\rho}_y v\hat{\rho}_y-\hat{\rho}_z v\hat{\rho}_z\right]\right)\,\mathrm{d}t\right)$$

where $\hat{\rho}_i$ are defined in equation (17) and

$$\hat{\rho}_i v\hat{\rho}_i(t)\equiv\int_{rr'}\mathrm{d}^3r\;\;\mathrm{d}^3r'\;\;\hat{\rho}_i(r,t)v(r-r')\hat{\rho}_i(r',t). \tag{44}$$

We can now apply the usual relativistic HST given in equation (19) to give

$$\exp\left(-\frac{\mathrm{i}}{\hbar}\hat{H}T\right)=\int \mathrm{D}\sigma_{\mathrm{c}}\,\mathrm{D}\sigma_x\,\mathrm{D}\sigma_y\,\mathrm{D}\sigma_z\;\tilde{G}(\sigma_{\mathrm{c}})\tilde{G}(\sigma_x)\tilde{G}(\sigma_y)\tilde{G}(\sigma_z)$$
$$\times\exp\left(-\frac{\mathrm{i}}{\hbar}\int_{t=0}^{T}\mathrm{d}t\;\left[\sum_{i,s_i}\epsilon_{i,s_i}a^{\dagger}_{i,s_i}a_{i,s_i}+\mathrm{i}v\sigma_{\mathrm{c}}\hat{\rho}_{\mathrm{c}}-v\sigma_x\hat{\rho}_x+\mathrm{i}v\sigma_y\hat{\rho}_y-v\sigma_z\hat{\rho}_z\right]\right)$$

where

$$\tilde{G}(\sigma_i)\equiv\exp\left(-\frac{1}{2}\frac{\mathrm{i}}{\hbar}\int_{rr'}\mathrm{d}^3r\;\;\mathrm{d}^3r'\;\int_{t=0}^{T}\sigma_i(r,t)v(r-r')\sigma_i(r',t)\;\mathrm{d}t\right). \tag{45}$$

Now identifying $\mathrm{i}v\sigma_{\mathrm{c}}\equiv e\phi^{\text{old}}$, $v\sigma_x\equiv ecA_x^{\text{old}}$, $v\sigma_y\equiv ecA_y^{\text{old}}$, $v\sigma_z\equiv ecA_z^{\text{old}}$ and applying the gauge transformation (42) we obtain

$$\mathrm{e}^{-(\mathrm{i}/\hbar)\hat{H}T}=\int \mathrm{D}\sigma_{\mathrm{c}}\,\mathrm{D}\sigma_x\,\mathrm{D}\sigma_y\,\mathrm{D}\sigma_z\;\tilde{G}(\sigma_{\mathrm{c}})\tilde{G}(\sigma_x)\tilde{G}(\sigma_y)\tilde{G}(\sigma_z)$$
$$\times\exp\left\{-\frac{\mathrm{i}}{\hbar}\int_{t=0}^{T}\mathrm{d}t\left(\sum_{i,s_i}\epsilon_{i,s_i}a^{\dagger}_{i,s_i}a_{i,s_i}-\left[v\sigma_x(t)+c\int_{t'=0}^{t}\frac{\partial}{\partial x}\mathrm{i}v\sigma_{\mathrm{c}}(t')\,\mathrm{d}t'\right]\hat{\rho}_x\right.\right.$$
$$+\mathrm{i}\left[v\sigma_y(t)+c\int_{t'=0}^{t}\frac{\partial}{\partial y}\mathrm{i}v\sigma_{\mathrm{c}}(t')\,\mathrm{d}t'\right]\hat{\rho}_y$$
$$\left.\left.-\left[v\sigma_z(t)+c\int_{t'=0}^{t}\frac{\partial}{\partial z}\mathrm{i}v\sigma_{\mathrm{c}}(t')\,\mathrm{d}t'\right]\hat{\rho}_z\right)\right\}. \tag{46}$$

On performing the Wick rotation, $\beta=\mathrm{i}T/\hbar$, $\tau=\mathrm{i}t/\hbar$, $\tau'=\mathrm{i}t'/\hbar$, this leads us to the representation of the density matrix as

$$\mathrm{e}^{-\beta\hat{H}}=\int \mathrm{D}\sigma_{\mathrm{c}}\,\mathrm{D}\sigma_x\,\mathrm{D}\sigma_y\,\mathrm{D}\sigma_z\;G(\sigma_{\mathrm{c}})G(\sigma_x)G(\sigma_y)G(\sigma_z)$$

$$\times \exp\left\{-\int_{\tau=0}^{\beta} d\tau \left(\sum_{i,s_i} \epsilon_{i,s_i} a^{\dagger}_{i,s_i} a_{i,s_i} - \left[v\sigma_x(\tau) + c\hbar \int_{\tau'=0}^{\tau} \frac{\partial}{\partial x} v\sigma_c(\tau')d\tau'\right]\hat{\rho}_x + i\left[v\sigma_y(\tau) + c\hbar \int_{\tau'=0}^{\tau} \frac{\partial}{\partial y} v\sigma_c(\tau')d\tau'\right]\hat{\rho}_y - \left[v\sigma_z(\tau) + c\hbar \int_{\tau'=0}^{\tau} \frac{\partial}{\partial z} v\sigma_c(\tau')d\tau'\right]\hat{\rho}_z\right)\right\}. \quad (47)$$

We denote the one-electron propagator in equation (47) by $\hat{U}'(\sigma)$. We see that the scalar potential ($\hat{\rho}_c$-term) has been eliminated and that the effective vector potential is real. This is beneficial because it removes some of the problems associated with an imaginary auxiliary field.

The non-relativistic generalization of this relativistic $\phi = 0$ representation of the electric and magnetic fields is actually equivalent to the representation used in the non-relativistic case by Chang [11]. Although using the above representation leads to a single-electron propagator $\hat{U}'(\sigma)$ which contains a *real* 4-potential, the properties of such a representation do not appear to be as convenient as the simple 4-field case described earlier in section 3 when we perform numerical calculations. In particular, the size of the correction to the vector potential in equation (42), given by

$$A'(r, t) = \int_{t'=0}^{t} \nabla\phi(r, t')\, dt'$$

grows as $N^{1/2}$ with increasing number of Trotter time steps N, and hence increases in magnitude with increasing time. Also, since $\nabla \equiv ik$ in reciprocal space, the $\nabla\phi$ term in equation (47) means that the coefficients of the large Fourier components of ϕ are enhanced compared to the coefficients of the smaller Fourier components, leading to new fields which oscillate more quickly in space than the fields in the 4-field representation given in equation (19). Such a problem indicates that we may have to take a very large number of plane-wave coefficients for our wavefunctions before we achieve convergence of $E(\beta)$ with increasing number of plane waves. In fact, attempts at numerical calculations using the projection method described in equations (31)–(33) show that we do indeed face such problems when working numerically in the $\phi = 0$ gauge. Numerical results for such a representation are recorded in figures 3 and 4 for basis sets of 343 plane waves and 125 plane waves respectively. The results are similar to those in figures 1 and 2 for the 4-field gauge.

Because of the form of $E(\beta)$ given in equation (33) we can expect a curve of the form $E(\beta) = a(1 - e^{-b\beta})$, where a and b are constants (i.e. an exponential decay,) to fit the data at large enough β. In this way we can hope to extrapolate the results to $\beta = \infty$ in a meaningful way. Indeed, for a basis set of just 27 plane waves, the error bars are small enough to allow a least-squares fit of this form to the data. These results are given in figure 5, and show that the extrapolated values of $E(\beta)$ as $\beta \to \infty$ are similar for both the 4-field (equation (19)) and $\phi = 0$ (equation (47)) gauges described above. The discrepancy between the two graphs can be put down to the small number of plane waves used. For one particular point we have briefly investigated the convergence of $E(\beta)$ with $\Delta\tau$. In fact we find that the value of $\Delta\tau$ chosen for the graph is indeed small enough for any errors due to its non-zero size to be smaller than the statistical errors obtained in the AFQMC calculation. Unfortunately, increasing the number of plane waves used in the basis set leads to an increase in the statistical fluctuations as illustrated in figures 1 to 4. Hence a such a

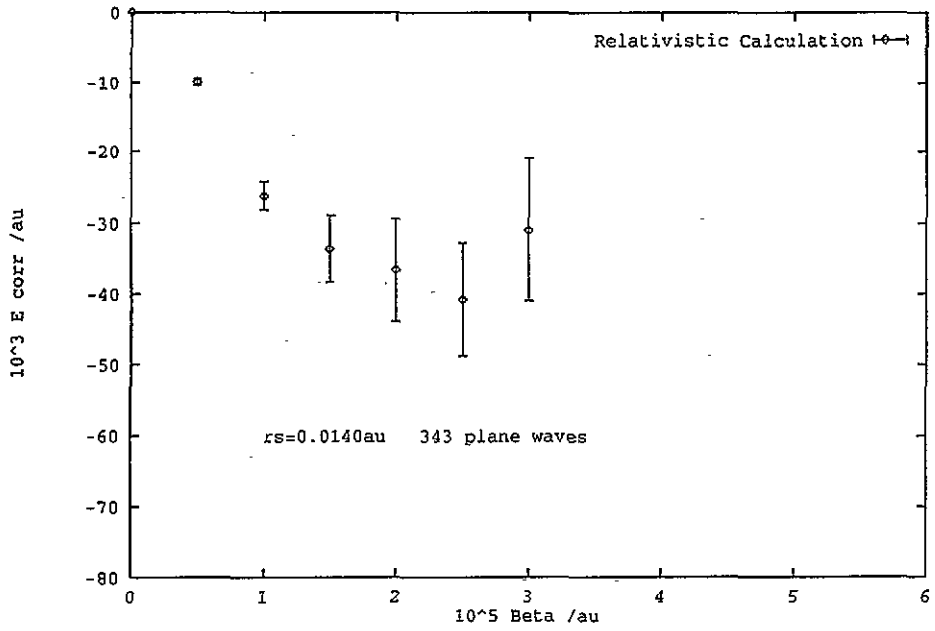

Figure 3. Relativistic AFQMC calculations of correlation energy E_c against β for a two-electron system at density $r_s = 0.0140$, using a basis set of 343 plane waves and the real-field representation in equation (47). $\Delta\tau = 2.5 \times 10^{-6}$.

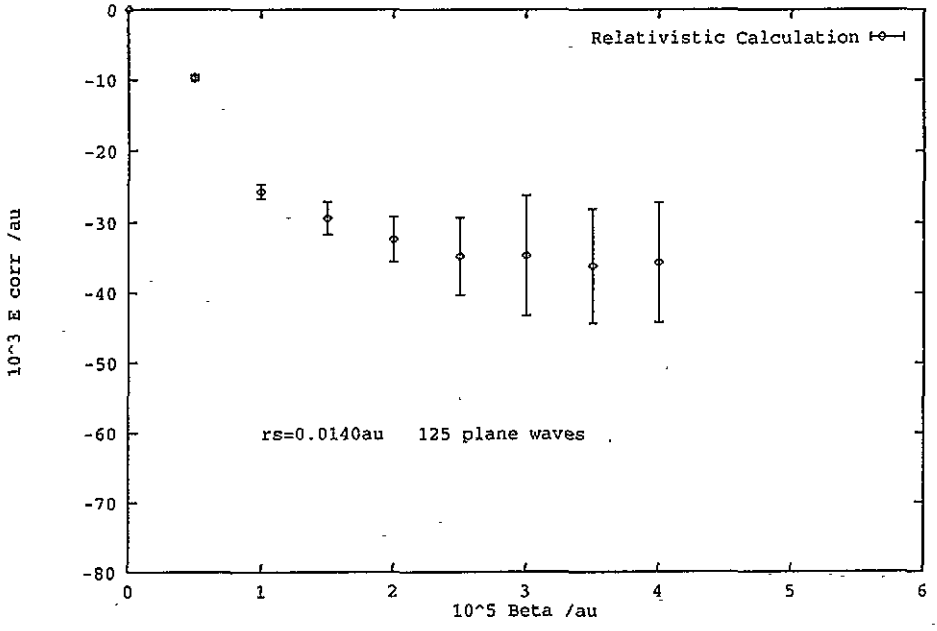

Figure 4. Relativistic AFQMC calculations of correlation energy E_c against β for a two-electron system at density $r_s = 0.0140$, using a basis set of 125 plane waves and the real-field representation in equation (47). $\Delta\tau = 2.5 \times 10^{-6}$.

direct comparison of the two gauges is not possible for a system described by more plane waves. Nevertheless, the results suggest that within the statistical error the two different

gauges give the same results, as we should expect.

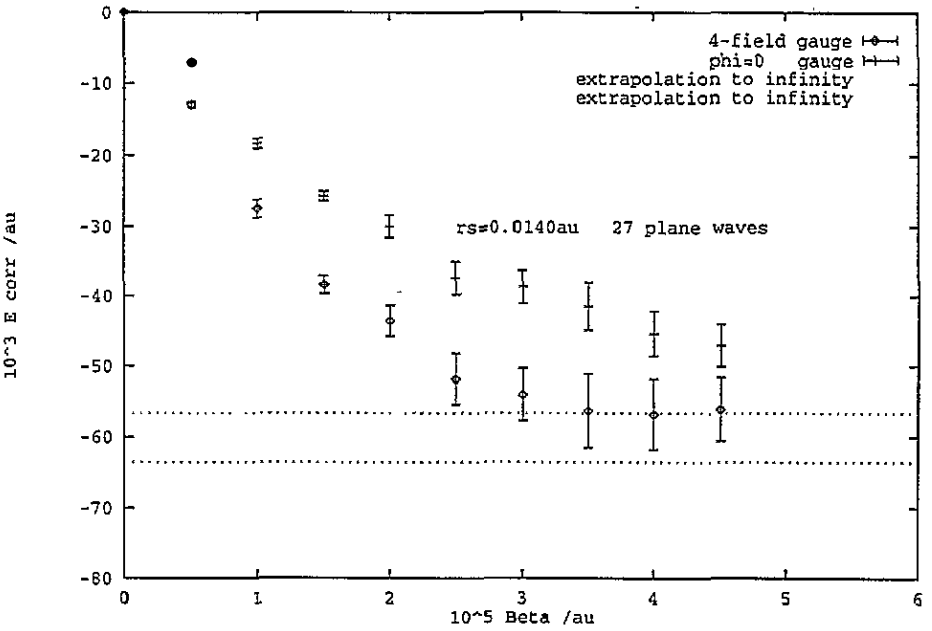

Figure 5. Relativistic AFQMC calculations of correlation energy E_c against β for a two-electron system at density $r_s = 0.0140$, using a basis set of 27 plane waves and both the 4-field representation in equation (19) and the real-field representation in equation (47). The points have been extrapolated to $\beta = \infty$ by considering a simple exponentail decay. $\Delta\tau = 2.5 \times 10^{-6}$.

7. Discussion and conclusions

Firstly we wish to comment on the significance of the numerical results. We clearly see from figure 1 that the non-relativistic and relativistic cases produce different results, with the addition of relativity significantly lowering the ground-state energy. Statistical errors, however, are large, and although both curves are beginning to tend to limits, in the relativistic case there is a large degree of uncertainty. Calculations were performed for up to (typically) 5000 σ-fields per point on the graph. The Monte Carlo acceptance rate was large in all cases, being indicative of the small value of r_s at which we are working. Calculations took typically a few CRAY hours per point on the graphs. The Monte Carlo acceptance rate was very close to unity for all the points, suggesting that a better way of sampling the fields exists. This possibility has not yet been explored.

We can compare these results with those of Ramana and Rajagopal [9], who have calculated exchange–correlation energies for jellium using a ring-diagram approximation. They obtain the result $\epsilon_c = -280 \times 10^{-3}$ au, which compares with our Monte Carlo value of $\epsilon_c = -25(\pm 5) \times 10^{-3}$ au (for 343 plane waves,) where ϵ_c is the correlation energy per particle. We see that we have recovered only of the order of one tenth the correlation of a proper jellium by using our repeated two-electron jellium. We believe that this is principally a size effect, namely we would require many more electrons in order to obtain a sensible value; at the present time this is not feasible due to the computer expense involved.

Secondly, we observe that the case of the fermion sign problem is more serious than in the non-relativistic case. Since the correlations of the system increase as r_s is increased

we expect the auxiliary-field method to perform less well at higher r_s, due to the larger fluctuations in the σ-field needed to take into account the correlations. In fact, we find that this is the case. However, the onset of the sign problem occurs at much smaller r_s for the relativistic case than for the non-relativistic case. Indeed, for $r_s = 4$ (where relativistic effects would be negligible) the relativistic method is unable to produce any meaningful result due to the fermion sign problem, whereas the non-relativistic method works well. This effect must be due to the presence of the three 'vector potential'-like fields, σ_x, σ_y, σ_z, whose net effect must average to zero in the non-relativistic régime but in fact produce large fluctuatons.

In short, we have generalized the HST to the relativistic case and have applied it in a Monte Carlo calculation to a two-electron jellium system. Such a method is implicitly exact, and removes the need for perturbation theory approximations, but is computationally expensive. However, we have discovered that the HST provides a very natural representation for the density matrix operator $\exp(-\beta\hat{H})$, closely related to Feynman's formulation of QED. This suggests that a search for more convenient auxiliary fields is unlikely to be successful. We have found that gauge freedom allows us to generate any number of different auxiliary-field representations. In particular, we have shown how the problematic imaginary scalar field arising from the natural 4-field representation of the density matrix can be eliminated in favour of a real vector field.

References

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